An optimized algorithm for the prediction of the water emptying time on BPNN

BY

Hanfeng Zhai, [a] Kai Wang, [b] Zhenyu Liu [c]

a. *Department of Mechanics, School of Mechanics and Engineering Science, Shanghai University, Shanghai, China*

b. *Process Equipment and Control Engineering, College of Energy Engineering, Zhejiang University, Zhejiang, China*

c. *Mechanical Engineering, School of Mechanical Engineering, Zhejiang University, Zhejiang, China*

E-Mail: frankzhai0@gmail.com; 3170103040@zju.edu.cn; riofredi@outlook.com

RESEARCH

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Dr. Reza Alam

CONTENT

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Abstract

The water discharge problem is a classic fluid mechanics problem yet hard to resolve due to its complex nature involves water-air interactions that generate air bubbles and vortex. Here, we analytically show that for water discharge in a square pipe, the water emptying time is quadratically proportional to water height and pipe length, and the solution is distributed on a "solution surface" in the $t - h - l$ space. Also, we found out that the water emptying time is shorter with bigger angles, and the water discharge rate is the highest for the Nongfu spring bottle and lowest for the Pocalri bottle. We explain such by bottle shape, depicted by the bottleneck shape and bottle-body trough. We qualitatively show that with a bottle shape depicted by $n > 1$ with our equation, or with a trough on the bottle-body, there is more likely to generate vortex and friction to slow the discharge. For what is more, the bottle-body trough plays a major in our approach. Inspired by the preceding approaches to solving fluid mechanics problems with machine learning, specifically using neural networks, we build a regression model based on our experimental data of the water discharge with BPNN to obtain the satisfied network through a strategy we called "Lucky-Draw". We obtain that for our data the best BPNN parameters are: $\xi = 1$ and $\alpha = 10^{-3}$. Henceforth, we generate the satiated network with our algorithm shows good accuracy. We also implement a randomly generated dataset to get a prediction from our network.

Keywords: fluid mechanics; water discharge problem; BPNN; machine learning

1 Introduction

The water discharge is a phenomenon that is rather common in our daily life and a classic fluid mechanics problem. Such a problem, while may seems simple and common, is difficult to resolve due to its complex essence. The two-phase flow of water and air involves slippery water-air interactions and inter-surface contact, which requires a complicated mathematical model [1]. Therefore, a purely analytical approach is time-consuming and inefficient. For what is more, preliminary experimental approaches are more widely adopted for students to investigate [2] and statistical estimation of the experimental data could provide a valuable message as to elucidate the water discharge mechanism [3]. The process of explaining such problem with experimental approaches is presented as examples for analysis by H. Mayer [4], who coupled with the experimental data with the traditional mathematical model and contends that the water emptying time is positively proportional to bottle volume, maximum diameter, bottle height and negatively proportional to neck diameter, which is similar to out approaches.

However, with the fast-growing technology, due to its efficiency and viability, simulation is a more widespread approach nowadays, especially for fluid mechanics problems. As mentioned in the previous paragraph, the two-phase flow is a knotty issue engaged in the water discharge, while Liu *et al*. [5] present a CFD approach for the macroscopic water discharge for the flood. For what is more, the numerical approach also elucidated that the specific bottle dropping water discharge problems involves a generation of an air bubble between in the bottleneck area, the pressure around such area is wavy with time and the fluctuation is more intense with the bigger bottle outlet diameter [6]. Furthermore, the air bubble involved is one of the most important characteristics in the water discharge problem, as studied both from the dynamical perspective and the vibrational perspective ([7], [8]). Subsequently, other approaches such as image estimation with high speed camera is also implemented in investigating such a problem and provide valuable information about how the air bubble evolves [9].

Aside from the analytical, experimental, numerical, and image approaches, currently, machine learning is widely adopted in the study of fluid mechanics. Specifically, neural networks are especially suitable for studying complex fluid mechanics problems to reveal the mechanisms beneath the complex experimental data. In 1989, the NASA scientists already provide a feasible approach using an algorithm to predict the noise of a NACA airfoil as a regression model [10]. Later on, in the 21st century, neural network approaches have been implemented on the same database and all generate satiated results ([11], [12]).

Inspired by such exciting and promising results, we implement the neural networks approaches on the water discharge problem, to see whether we can obtain satisfying results as presented with the traditional approaches. Our basic strategy is to consider the water discharge experimental data as a regression model, in which the bottle's parameters and angles are input data and the water emptying rate is the output data. We implement a BPNN with our algorithms and predict the water emptying time compared with our experimental data to check the accuracy.

2 Method

2.1 *Problem formulation*

As discussed in §1, the water discharge problem is a classic fluid mechanics yet rarely studied in modern scientific researches. The problem, while may seem simple and rather common in daily life, considering the complex two-phase fluid interaction and the interfacial problems involved between water and air, the problem is intricate and even difficult for simulations. Hence, a new strategy is being adopted, coupling statistics with fluid mechanics knowledge, one could discern certain scientific nature with the experimental approach.

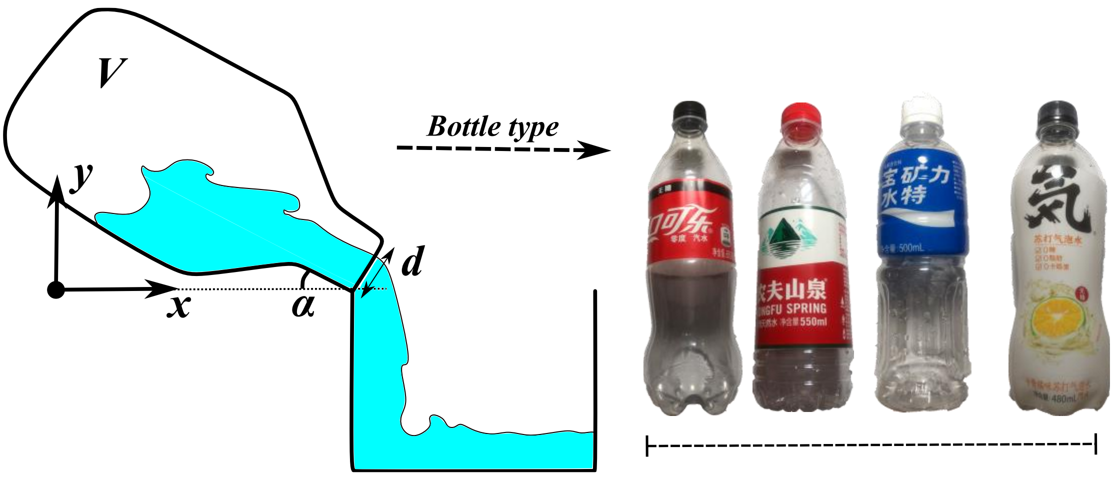

Fig. 1 Schematic illustration for the water discharge problem and the experimental method. Note that the bottles are named coke, Nongfu spring, Pocalri, soda bottle, from left to right.

The schematic view for the experiments is shown as in Fig. 1, in which we change four different types of bottles having different bottleneck diameter, volume, and shape; changing tilted angles, one could obtain different water emptying time. Here, we measure the time with the same parameter (i.e. angle, diameter, volume, etc.) for ten sets to increase the accuracy as possible. Note that the angles are set to be at three values, i.e. 30, 45, 60, in degrees.

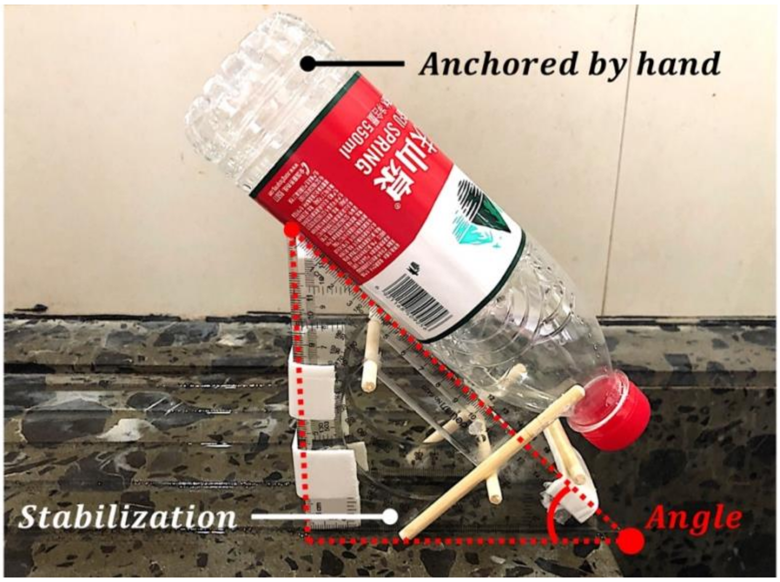

Fig. 2 Picture for the experimental setup.

Here, we present a picture showing how we approach the experiment in Fig. 2. In the process, we control the angle with specific rulers and anchor the lower part of the bottle with our hands. We measure the emptying time when water started to drop out of the bottle and measured ten times with the same groups of parameters. The data is recorded matched with each's corresponding parameters.

2.2 *Mathematical model*

Here, we try to present a way to obtain the analytical solution as a simplified model for the water discharging problem. Now we consider a horizontal bottle as shown in Fig. 3, with a square cross-section of side length *a*. Provided that the water is flowing out at a steady-state and the water-air interaction is neglected.

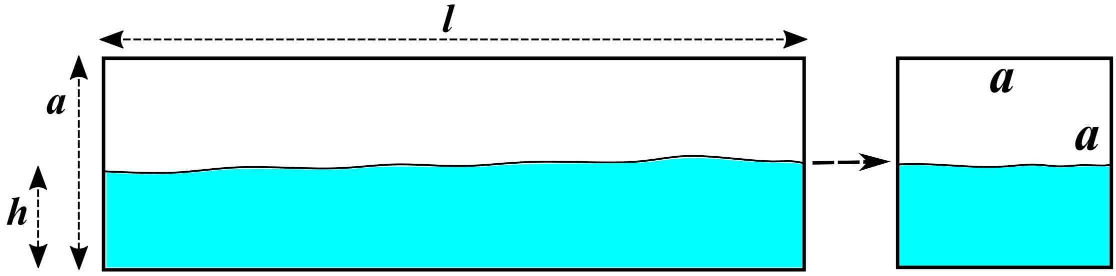

Fig. 3 Schematic view for the water flow problem, in assumed conditions.

Now let us consider the momentum and the flow volume of the water:

$$\begin{cases} \rho g \dfrac{h}{2} \cdot ah \cdot dt = dm \cdot V = ahdx\rho \cdot \dfrac{dx}{dt} & (1) \\ dQ = dh \cdot l \cdot a = ah \cdot dx & (2) \end{cases}$$

Where $dx = \frac{dhl}{h}$ in (2).

Substitute such into Eq. 1:

$$\frac{gh}{2} = \frac{dx \cdot dx}{dt \cdot dt} \tag{3}$$

Which can be reduced to

$$\sqrt{\frac{gh}{2}} = \frac{dx}{dt} = \frac{ldh}{hdt} \tag{4}$$

Hence, one can deduce the water discharge time:

$$dt = \frac{ldh}{h}\sqrt{\frac{2}{gh}} \tag{5}$$

Here, we integrate Eq. 5, the water emptying time can thence be calculated as

$$\int dt = \int \frac{1}{h}\sqrt{\frac{2}{gh}}dh \tag{6}$$

Thence, the emptying time is obtained:

$$t = -2\sqrt{\frac{2}{g}}lh^{-\frac{1}{2}} + C \tag{7}$$

Where C is an indeterminate constant.

Based on our analytical solution (Eq. 7), we can provide a visualization as shown in Fig. 4. Although the model is greatly reduced and based on very special conditions, the solutions can still provide decent guidelines for our estimation of the water discharge problem.

As it is shown in Fig. 4, in the solution space ($t - h - l$), all the solutions are concentrated on a surface that I nominated "Solution surface". The height and length are linearly proportional to each other; the emptying time has a quadratic relation with water height and length. For what is more, as the constant changes, the solution “steepness” or shape is not changed in the solution surface.

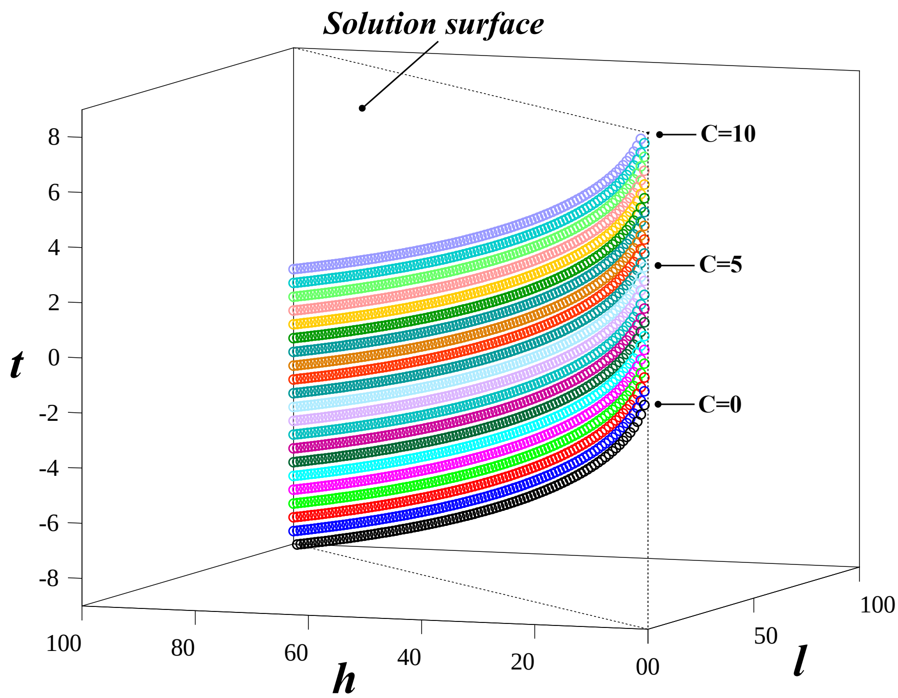

Fig. 4 Visualization of the analytical solution corresponding water emptying time with length and water height.

2.3 *Algorithm approach*

As mentioned in §2.1, we adopted an experimental method obtaining a $[12 \times 4]$ database. Notwithstanding, as given in the latter chapter §3.1, the water bottleneck’s shape and bottle-body’s trough also may influence the water discharge rate. Hence, we consider such two attributes as: if water bottleneck shape function parameter $n > 1$, then the value is 1, else 0; if water bottle-body has a trough, then the value is 0, else 1. Henceforth, we expand the database to $[12 \times 6]$.

Estimating the database one can discern that the calculation of the water emptying time can be regarded as a regression model, in which the input data involves

5 sets: bottle type, bottle volume, … as shown in Fig. 5. The water emptying time is calculated as the mean value.

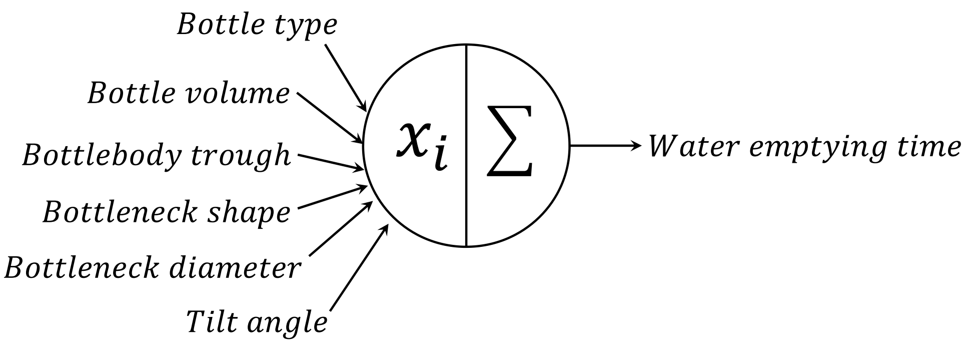

Fig. 5 Illustration for the regression problem based on the experimental data.

Algorithm 1: Determining the Parameters of Original BPNN

Set the initial value of sum of the determining factor $R^2_{\text{sum}} = 0$; and sum of the relative error $\varepsilon_{\text{sum}} = 0$.
For a loop running with 10^3 iterations:
  Clear all the remaining values of the last iteration;
  1: Importing and operating the data.
  2: Generate the network:
    Change the specific parameters:
      i. Set the neuron numbers $\xi \to$ change from 1 to 20.
      ii. Set the training epochs $= 10^5$.
      iii. Set the training goals $= 10^{-3}$.
      iv. Set the learning rate $\alpha \to$ change from 10^{-1} to 10^{-5}.
    Training the data with given parameters and creating simulation.
  3: Calculate the results:
    The sum of determining factor $R^2_{\text{sum}} = R^2_{\text{sum}} + R^2$, the sum of the relative error $\varepsilon_{\text{sum}} = \varepsilon_{\text{sum}} + \varepsilon$.
    The mean value of R^2 and ε is calculated by $\frac{R^2_{\text{sum}}}{\text{Iterations}}, \frac{\varepsilon_{\text{sum}}}{\text{Iterations}}$.
    Calculate the CPU running time t_{run}
End the loop.

There are various ways of building a regression model and providing solutions. The simplest one is a linear regression model. However, considering the relatively few data and the complex nature of such a problem as mentioned in §2.1, such a model might not provide accurate predictions. Here, we provide a neural network method, for the prediction of the water emptying time. A simple BPNN parameter deciding process is shown as in Algorithm 1.

As shown beyond, Algorithm 1 gives an approach of finding the best neuron numbers ξ and learning rate α, which are the two parameters that might greatly influence the network's performance, for the generation of the neural network with best efficiency and accuracy.

Algorithm 2: Obtain the BPNN model

For a loop running with 10^5 iterations:
- Clear all the remaining values of the last iteration;
- 1: Operating the data:
  - Import the water discharge experimental data to define the input and output data, and set the training and testing sets.
  - Normalize the input dataset.
- 2: Generate the network:
  - Set the given parameters obtained from Algorithm 1.
  - Training the data with given parameters and creating simulation.
- 3: Calculate the results:
  - Obtaining errors and deciding parameter R^2;
  - Outputs the results as comparing the testing data and simulation results, and calculate the relative error ε.
- 4: Generate a condition to break the loop:
  - If a value of R^2 that beyond 0.95 is detected, then plot the errors distribution and break the loop.

End the loop.

After obtaining the best parameters that fit the data for the BPNN with the highest performance, we need to generate the network satisfies our standard ($R^2 > 0.95$) as shown in Algorithm 2. Hence, we create a loop with a large circulation number (10^5 in our approach) to find such a condition. When the condition is detected, the loop is break and the results are obtained, which we nominate as "Lucky-Draw". Note that the calculation is carried out by Lenovo ThinkPad E480 with CPU: intel CORE i5 8th Gen. The code is running in MATLAB R2017A with system: Windows 10.

3 Results and discussion

3.1 *Experimental estimation*

Based on experimental operations as given in §2.1, we obtain results as shown in the following figures. To show the range and deviation of the datasets, we plotted the graphs as the form of a boxplot.

Here in Fig. 6, one observes that for the coke bottle, as the angle increases, the water emptying time evidently reduced. For what is more, the deviation is larger for the angle of 60, in degrees. Such results indicate that for the coke bottle, larger angles give a more discretized data distribution. This may cause by the air bubble or air-water interactions in an increasing steepness. While it also may cause by the specific shape of the coke bottle.

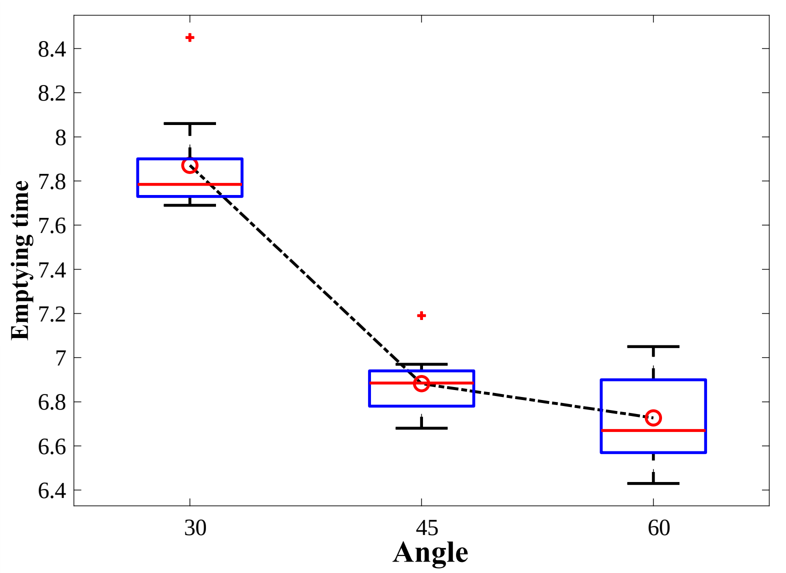

Fig. 6 The Emptying time-angle boxplot diagram of the coke bottle.

However, the same nature does not apply to the Pocalri bottle or the soda bottle as shown in Fig. 7 and Fig. 8. As shown, for Pocalri and soda bottle the emptying time does not show an evidently higher deviation with larger angles. Moreover, the error distribution does not increase eminently with bigger angles. Such results could be explained by the specific shape of the Pocalri and soda bottle. Notably, the emptying time dropping patterns both follows an approximately linear mode for Pocalri and soda bottle (Fig. 7 and Fig. 8), yet dropping either slower or faster for coke bottle and Nongfu spring (Fig. 6 and Fig. 9).

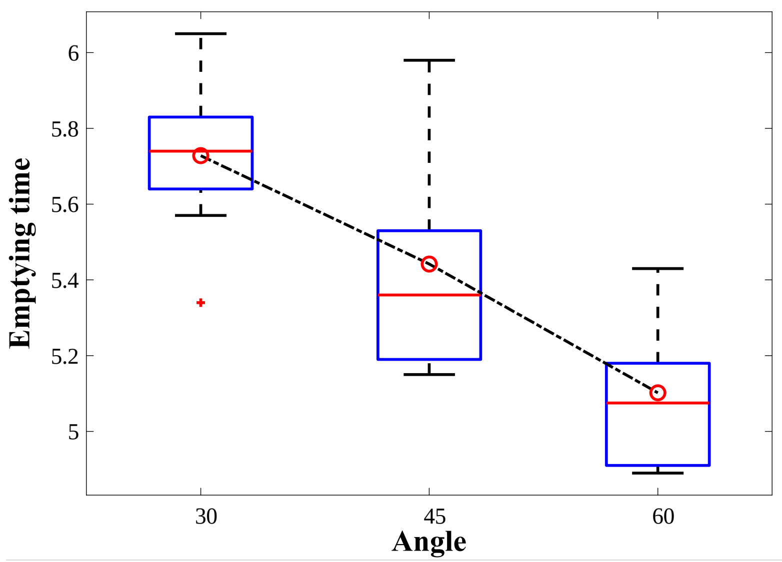

Fig. 7 The Emptying time-angle boxplot diagram of the Pocalri bottle.

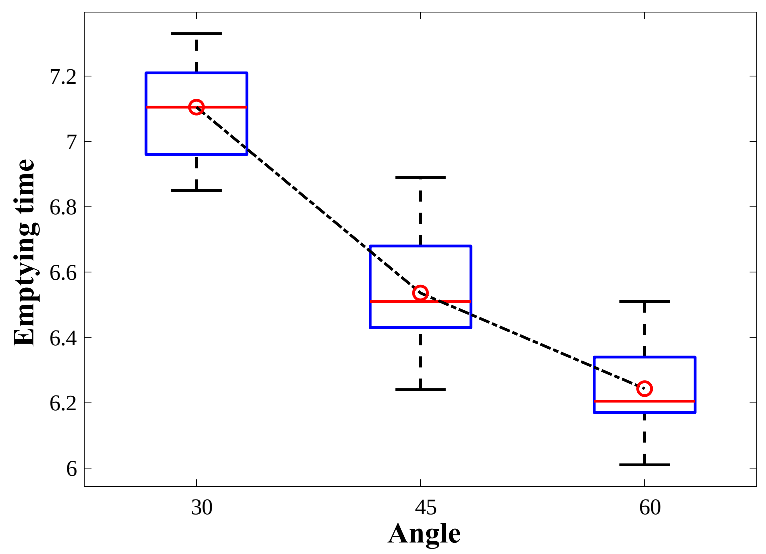

Fig. 8 The Emptying time-angle boxplot diagram of the soda bottle.

But if we neglect the emptying time dropping patterns, the data distribution is very similar for coke and Nongfu spring bottle. Both have an eminently higher deviation with the increasing angles, and both have a larger error bar with the increasing angles (Fig. 6 and Fig. 9).

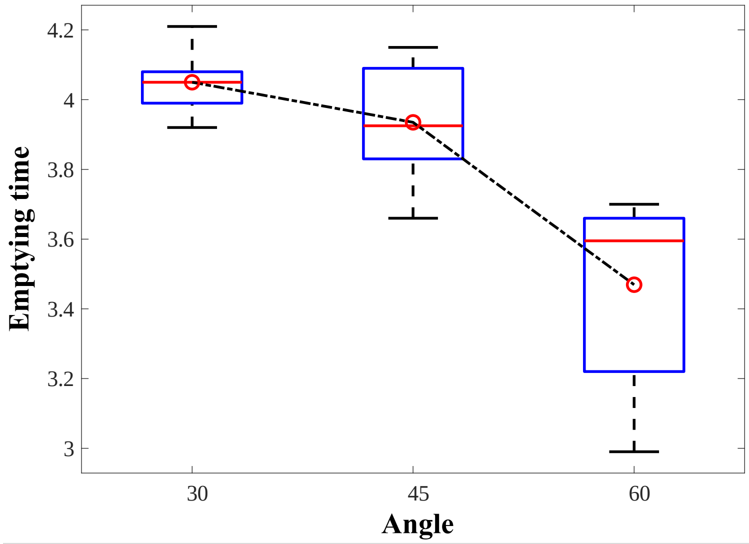

Fig. 9 The Emptying time-angle boxplot diagram of the Nongfu spring bottle.

From the previous discussions, we know that the bottle shape may play an important role in determining the water emptying time. To investigate such, we need to obviate the effect of the bottle volume difference. Henceforth, we define water discharge rate τ as the division of the water emptying time t to bottle volume V:

$$\tau = \frac{V}{t} \tag{8}$$

Here, Fig. 10 shows us how angle affects the water discharge rate for different types of bottles. From the relations, the water discharge rate is positively correlated with the angle. Notwithstanding, the Nongfu spring bottle has an evidently larger discharge rate than other types of bottles as shown. The Pocalri bottle has the least discharge rate comparing with others.

The bottle shape could provide guidelines for the explanation of such a discharge rate difference, which is shown in Fig. 11 and Fig. 12.

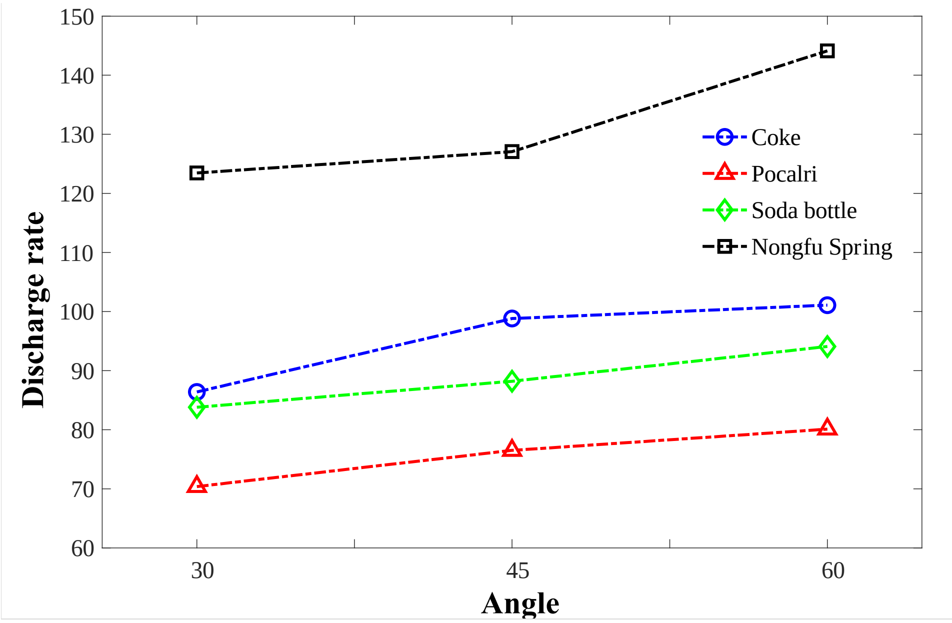

Fig. 10 The discharging rate calculated as a mean value comparing the four bottles.

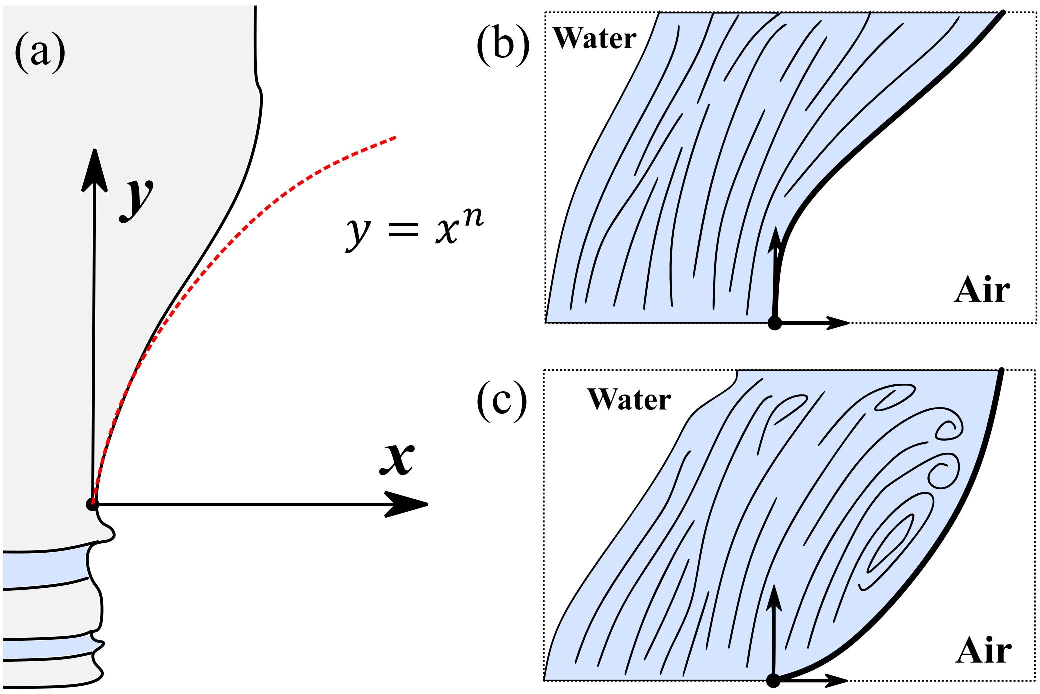

Fig. 11 Schematic of the provided explanation of the water discharge rate considering the bottleneck shape. (a) Basic strategy for mathematical description of the bottle shape. (b) The schematic of water emptying process when $n < 1$. (c) The schematic of water emptying process when $n > 1$.

In our studies, we try to depict that bottle shape with two main factors, the bottleneck shape and bottle-body trough. For the bottleneck shape, we try to delineate such with a function $y = x^n$ as shown in Fig. 11 . When $n > 1$, the bottle shape is shown as in Fig. 11, which is correlated with the bottle shape of coke. Such a shape indicates a smoother flow, or, with less vortex or flow friction due to its streamlined shape. When $n < 1$, the bottle shape is shown as in Fig. 11, where there is a larger possibility for flow the generate vortex and friction with the bottle inner surface. Such an effect might dissipate the energy and slower the water dropping process. The preceding theory might provide an explanation for the coke bottle has a higher discharge rate than Polcari and soda bottle. Yet the evidently higher discharge rate of Nongfu spring is not elucidated.

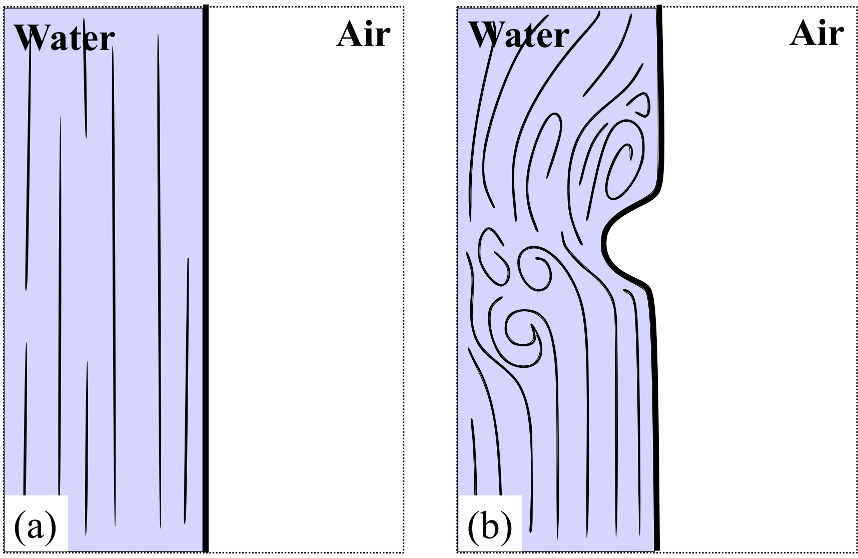

Fig. 12 Schematic of the provided explanation of the water discharge rate considering the bottle-body shape. (b) The schematic of water emptying process when the bottle-body has no trough. (b) The schematic of water emptying process when the bottle-body has a trough.

Observing the four bottle types, we find that both bottles have an evident trough on the bottle-body except the Nongfu spring. The bottle-body trough can create flow vortex and generate friction as shown in Fig. 12. Such a theory could explain why the Nongfu spring bottle has the highest water discharge rate. Moreover, coupled with experiments, we know that the bottle-body trough plays a more important role in influencing the water discharge rate.

Applied with the preceding theories, we could also explain why the Pocalri bottle has the lowest water discharge rate: the bottleneck shape could be depicted by $n > 1$ and has a larger n value than the other bottles. Such a shape generates vortex or even air bubbles that will robustly slow the discharge rate. For what is more, it has some trough on the bottle-body. Both characteristics will slow their discharge process. For the Nongfu spring bottle, although it does not have a streamline-liked bottleneck shape as coke does, its smooth bottle-body explains its fast discharge rate compared with the trough-shaped bottle-body of a coke bottle.

3.2 *BPNN algorithm*

Running the Algorithm 1, with the set learning rate 10^{-2} [2:iv], from the process [Step 2:i], we obtain how the neuron numbers ξ will influence the neural network's performance as shown in Fig. 13, Fig. 14, and Fig. 15.

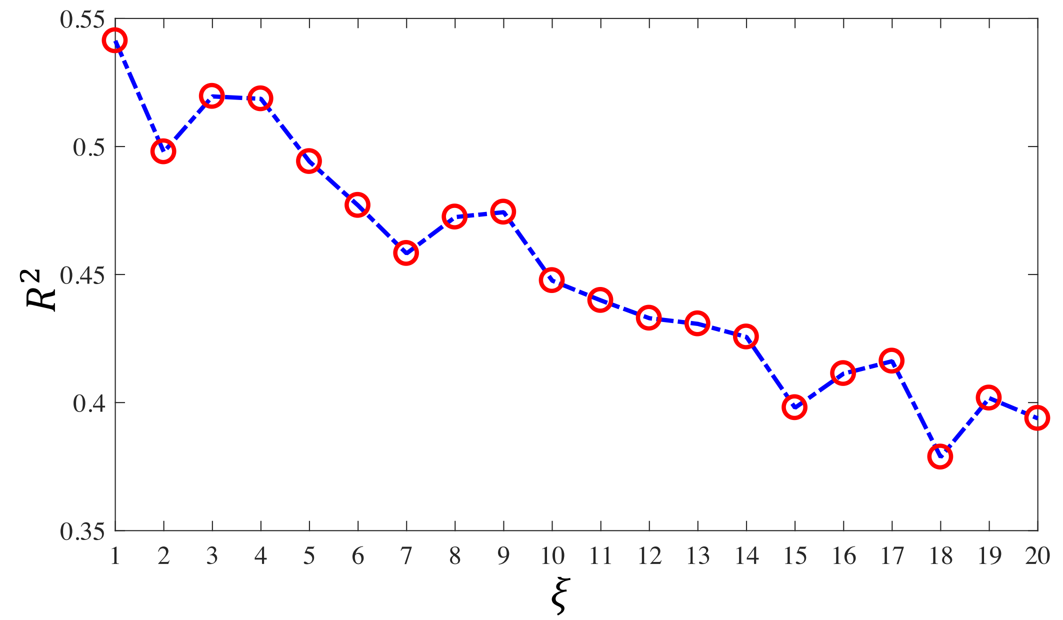

Fig. 13 The relations between the neuron numbers ξ to determining factor R^2.

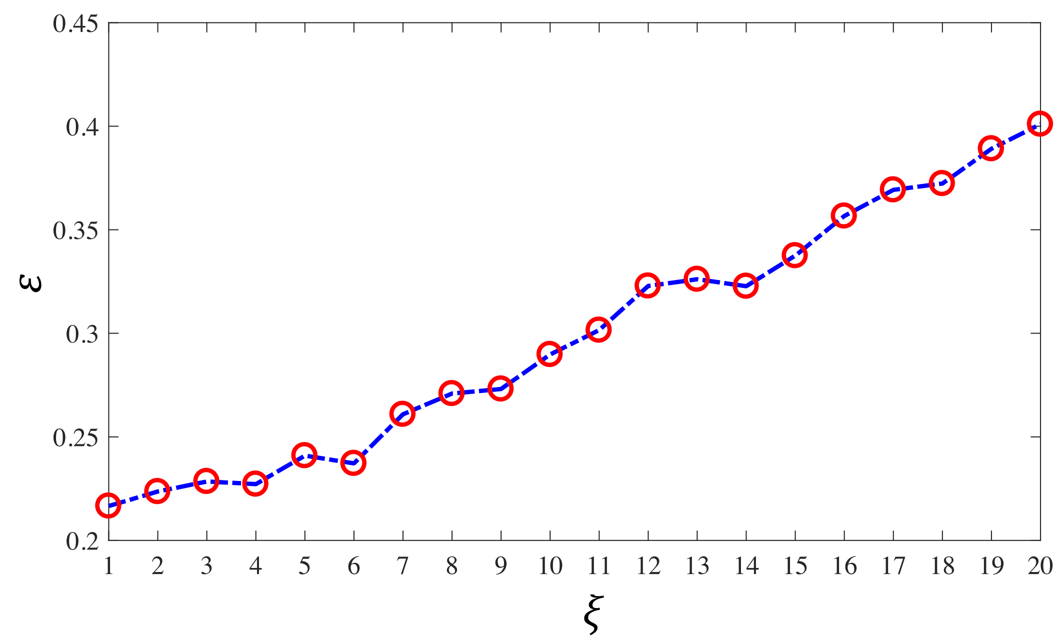

Fig. 14 The relations between the neuron numbers ξ to relative error ε.

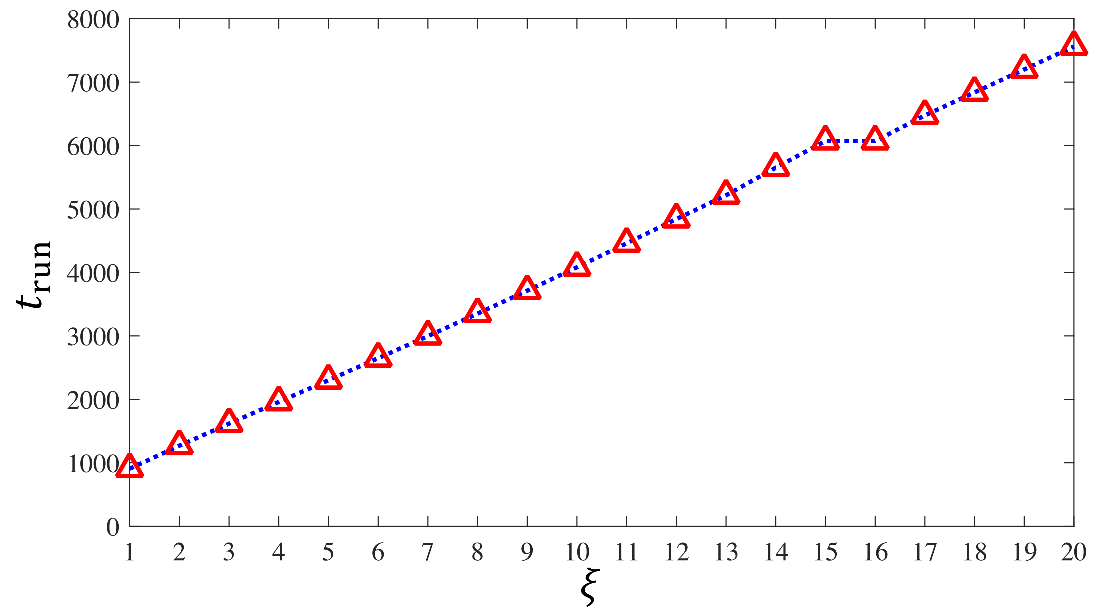

Fig. 15 The relations between the neuron numbers ξ to CPU time t_{run}.

Given that the equation for the determining factor R^2:

$$R^2 = N \cdot \sum T_{sim} \cdot T_{test} - \frac{(\sum T_{sim} \cdot \sum T_{test})^2}{(N \cdot \sum (T_{sim})^2 - (\sum T_{sim})^2) \cdot (N \cdot \sum (T_{test})^2 - (\sum T_{test})^2)} \tag{9}$$

Where N is the size of the input testing data matrix, T_{sim} is the simulation results, T_{test} is the testing samples.

The relative error ε is calculated as:

$$\varepsilon = \frac{\|T_{sim} - T_{test}\|}{T_{test}} \tag{10}$$

From the running results, we observe that when the neuron number $\xi = 1$ we obtain the neural network that has the biggest determining factor values (R^2), smallest relative error values (ε), and the least CPU running time (t_{run}), which is identified as the best neural network performance. Such a result does not match with our past experience of neural network training. We attribute such specific behavior to the small scale of the database. To be specific, due to we only have four types of bottle and three sets angle values, 12 sets is the most data that we can obtain from the longitudinal scale (Rows).

Following a similar strategy, given the neurons $\xi = 1$, we also run Algorithm 1 [2:iv] to determine the best learning rate α and obtain results as shown in Fig. 16 and Fig. 17.

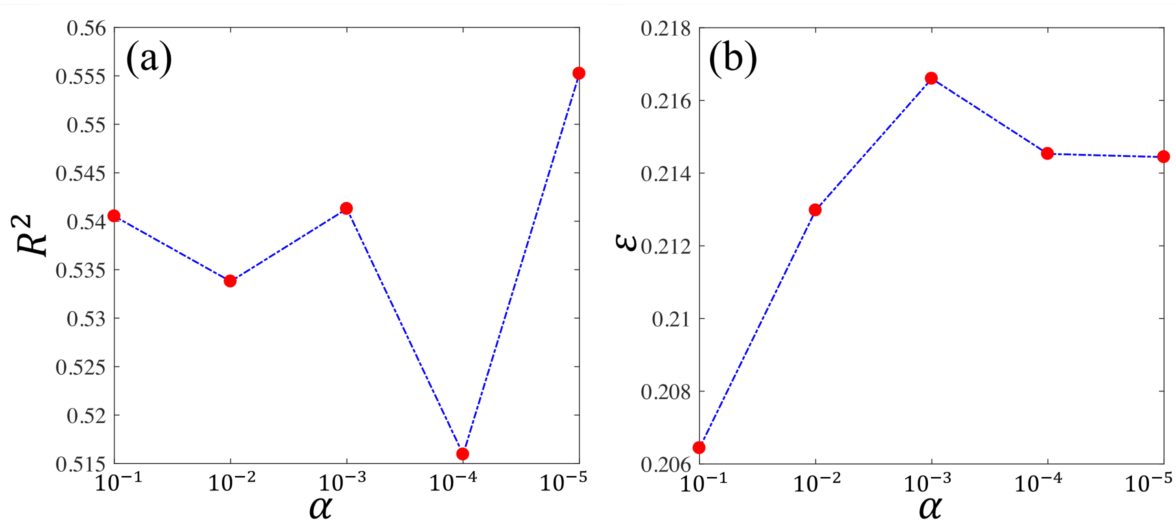

Fig. 16 The learning rate α effect on the network's performance. (a) The learning rate (α) – determining factor (R^2) diagram. (b) The learning rate (α) – relative error (ε) diagram.

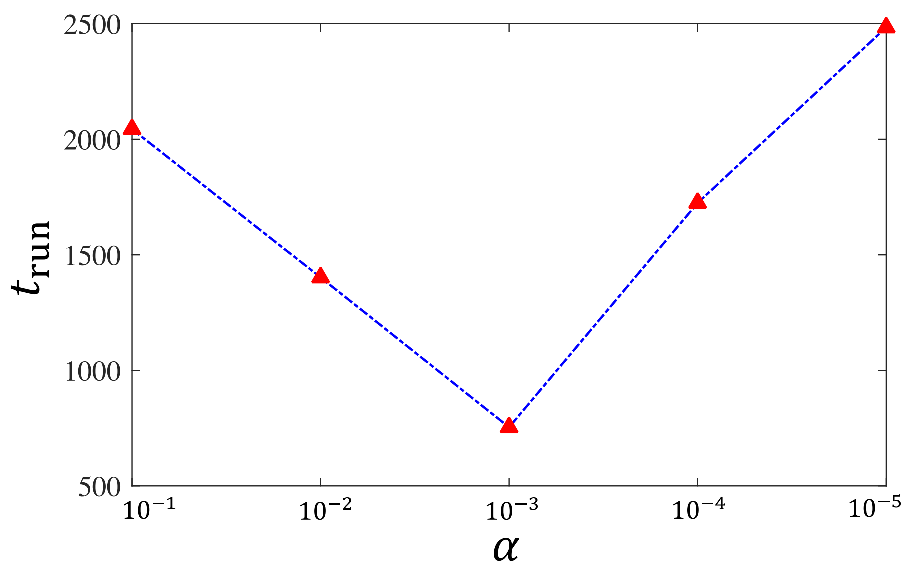

Fig. 17 The relations between the learning rate α to CPU time t_{run}.

From Fig. 16 we observe that both the determining factor R^2 and the relative error ε does not indicate a specific learning rate. Yet Fig. 17 indicates that when $\alpha = 10^{-3}$ we obtain the smallest CPU running time t_{run}. Such a phenomenon indicate that $\alpha = 10^{-3}$ generate a network that has a better performance.

Set the parameters $\xi = 1$ and $\alpha = 10^{-3}$, we now run Algorithm 2 to obtain the desired neural network, the results is shown in Fig. 18, Fig. 19, and Fig. 20.

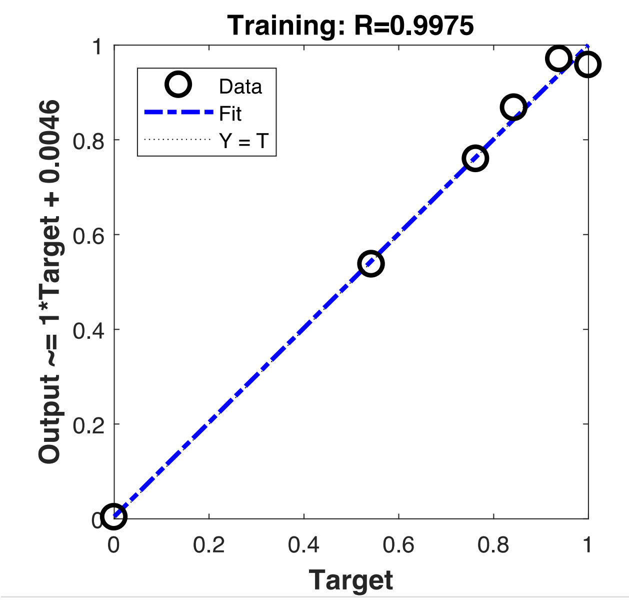

Fig. 18 The regression model of the generated network.

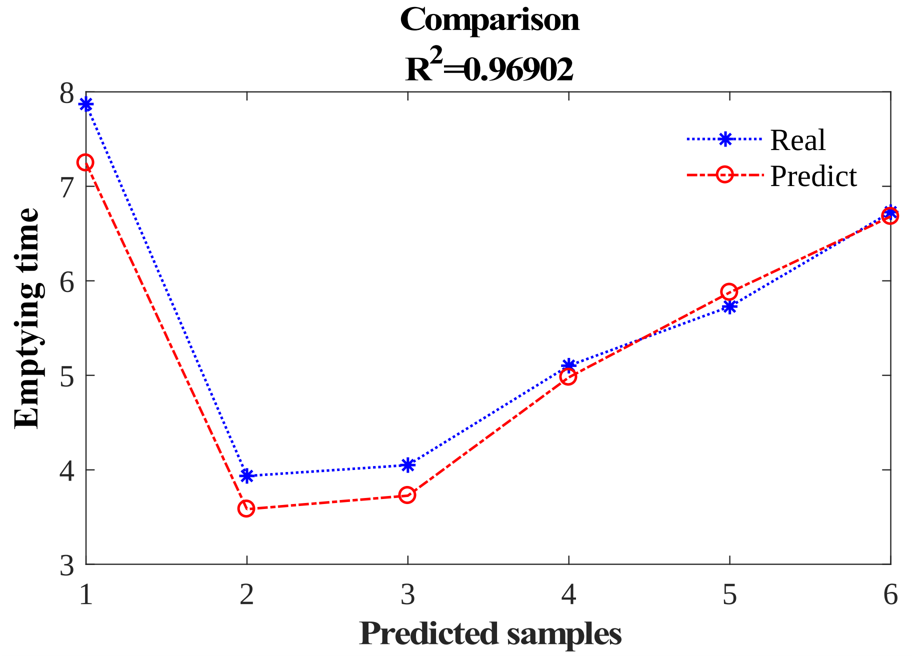

Fig. 19 The comparison between the testing samples T_{test} and the neural network's simulation results T_{sim}.

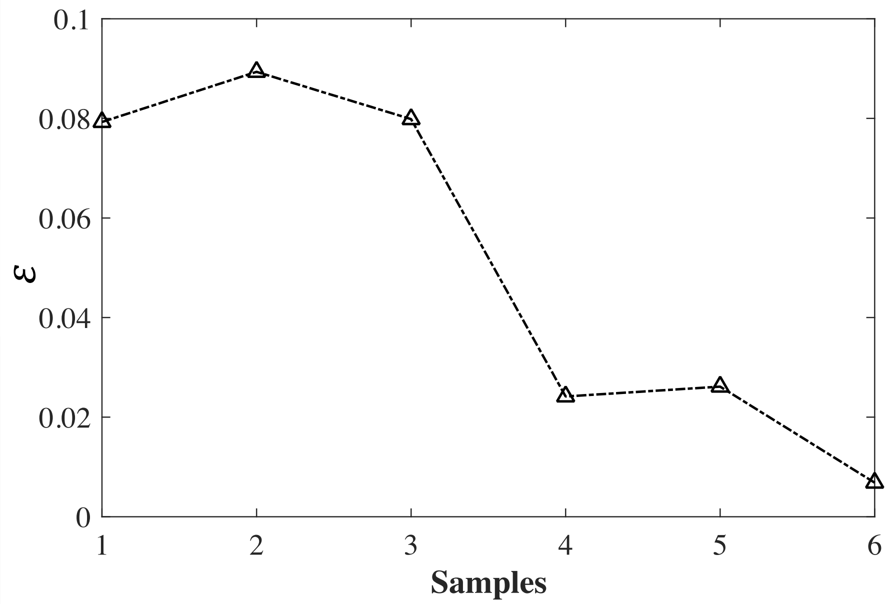

Fig. 20 The distribution of the relative errors ε with the testing samples.

Both Fig. 18 and Fig. 19 shows that the obtained neural network has valid performance, with determining factor $R^2 = 0.96902$ and small relative errors ε $\varepsilon < 0.1$. Here, we also provide an example: A Pocalri bottle with Bottleneck diameter: 2.5 cm; Volume: 500mL; Bottleneck shape: $n > 1$ with a bottle-body trough; with tilted angle $45°$. The predicted water emptying time: 3.2541s.

4 Conclusion

We investigate the water discharge problem three approaches, creating an experiment, and qualitatively estimate the experimental data, providing an analytical mathematical solution, and implement the experimental data on a BPNN model to predict water emptying time-based on our experimental parameters. We design experiments with two controlled parameters for the study: bottle type and angles as shown in Fig. 1, note that involve various parameters involved in bottle types. The bottle's body is anchored by rulers and hand as shown in Fig. 2. Subsequently, we present a water discharge mathematical model of a square pipe (Fig. 3). With the equation of momentum and the flow equation we reason out an analytical solution, pointing out that time is quadratically proportion to height and length, while the solution is distributed on a "solution surface" in the $t - h - l$ space as shown in Fig. 4. As introduced in §1, we consider the experimental database as a regression model, in which a schematic is shown in Fig. 5. To build such a model with the BPNN method, we provide two algorithms as shown in Algorithm 1 and Algorithm 2.

Experimentally we visualize our data of the water emptying time with regards to angles for four bottles as shown from Fig. 6 to Fig. 9. Such results show that both the bottles have shorter emptying time with larger angles. Howbeit for coke and Nongfu spring bottle, with larger angles, the data deviation is evidently larger with larger error bars (Fig. 6 and Fig. 9); yet such a pattern does not apply to Pocalri and soda bottle (Fig. 7 and Fig. 8). When we investigate the bottle shape effect on water discharge, we need to neglect the bottle volume, as we calculate the water discharge rate to depict the water dropping speed as shown in Eq. 8. Results indicate that the Nongfu spring bottle has the highest water discharge rate and the Pocalri bottle has the lowest. To explain such a phenomenon, we try to depict the bottle with two characteristics: the bottleneck shape and bottle-body trough. The bottleneck shape is depicted by $y = x^n$ as shown in Fig. 11. Qualitative analysis shows that with a $n > 1$ bottleneck shape water is more likely to be slowed when discharging (Fig. 11) and with a body trough water discharge are more likely to be slowed due to the vortex and friction (Fig. 12).

With the implementation of the Algorithm 1 of BPNN, we found out that for the experimental data, it is most efficient to take neuron numbers $\xi = 1$ (Fig. 13, Fig. 14, Fig. 15) and learning rate $\alpha = 10^{-3}$ (Fig. 16, Fig. 17) comparing the determining factor, relative error, and the CPU time of the neural network. With specified parameters, we run the BPNN model with Algorithm 2 and obtain the satiated network. Our obtained NN indicates good fitting (Fig. 18), acceptable accuracy with $R^2 = 0.96902$ and $\varepsilon < 0.1$ (Fig. 19 and Fig. 20). For what is more, as we input a randomly generated samples, we obtain a prediction from the network.

Our works applying BPNN with a small set of data are just preliminary approaches of combining machine learning with fluid mechanics, future works may involve optimization of the BPNN with the implementation of a bigger database.

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Authorship contribution statement

H. Zhai contributes to drafting the manuscript, providing the algorithms (BPNN) and conceive the results; K. Wang contributes to designing and carrying out the experiments; Z. Liu contributes to providing the analytical solution and carrying out the experiments.

Appendix. Code, data and supplementary materials

The code including Algorithm 1 and Algorithm 2, the raw and the operated database, and other related materials is uploaded on https://github.com/fzhai0/code.

Highlights

- Provide an analytical solution for a simplified water discharge problem.
- Experimentally show how the tilted angle influence the water discharge rate.
- Elucidate the bottle shape influence on the water discharge rate
- Provide a statistical method for the prediction of the water emptying time.