International Communications in Heat and Mass Transfer 76 (2016) 197–201

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Predicting bubble size and bubble rate data in water and in froth flotation-like slurry from computational fluid dynamics (CFD) by applying deep neural networks (DNN)☆

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ARTICLE INFO

Available online 26 May 2016

ABSTRACT

Accurate characterization of two phase bubbly flows is crucial in many industrial processes such as fluidized reactors, ore froth flotation, etc. The bubble size determines the rate at which components present in the gas phase are transferred to the surroundings and vice versa while bubble rate defines the appropriate bubbly flow regime occurring in the heterogeneous system. This research work employs deep neural networks (DNNs) to predict bubble size and bubble rate using data obtained from validated computational fluid dynamics (CFD) computations. Pure water and slurry (in conditions similar to those employed in mineral froth flotation) case studies are evaluated. It is found that the DNN can predict the CFD results accurately when using four hidden layers, describing discontinuities in the bubbly flow regime. The relative errors computed between the CFD data and the prediction obtained by the DNN is as low as 8.8% and 1.8% for bubble size and bubble rate, respectively. These results confirm that the DNN can be applied to sophisticated fluid dynamics systems and allow developing better control process strategies since once the DNN is trained critical variables can be computed very efficiently. The slurry case study, although restricted to the application of mineral froth flotation, can also be generalized to other industrial operations keeping the exact same procedure.

1. Introduction

Determining bubble size distribution and other characteristics of bubbly flows is a challenge and a necessity for a number of industrial operations such as mineral processing, oil industry, wine industry, wastewater treatment, fluidization reactors, bioreactors, etc. [1]. Particularly, in the field of mineral processing the search for new, improved and more accurate models to represent the efficiency of the froth flotation operation, one of the largest tonnage operations in the industry field, is still an ongoing process. Therein, it is widely accepted that the bubbly flow characteristics are key for a correct determination of the efficiency of the separation process and so far no analytical descriptions have been capable to gather all the information to understand the process. Although many models have been suggested as a possible representation of the froth flotation process and its sub-processes [2], they have proved to follow the trends the real systems exhibit. However, the uncertainty embedded in computing the efficiency of the operation is still an unresolved matter. Such uncertainty varies from 5 to 30% [3,4]. Computational fluid dynamics (CFD) tools are able to capture all complexities present in real froth flotation systems [5]. However, tracking the behavior of bubbly flows is an open problem.

The application of ordinary neural networks (NNs) has penetrated many applications fields dramatically and the mapping and prediction of fluid dynamic equations has been a highly fruitful field for scientific research [6]. One variation of NNs is the use of Deep Neural Networks (DNNs) which is one of the most recent developments in machine learning and represents a tremendous progress compared to the ordinary NN framework. DNNs are essentially neural networks with several (i.e. more than one) hidden layers that are pre-trained to reduce the limitations of the classic gradient based backpropagation training. Increasing the number of hidden layers improves the capability of the network to solve highly difficult, nonlinear and dynamic functions when compared to shallow networks. Nevertheless, to use a gradient-based

☆ Communicated by W.J. Minkowycz.
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http://dx.doi.org/10.1016/j.icheatmasstransfer.2016.05.031
0735-1933/

Nomenclature

a	Main or major bubble axis, [m]
b	Secondary or minor bubble axis (perpendicular to "a"), [m]
d_b	Bubble diameter, [m^3]
d_0	Inlet diameter for gas in the system, [m]
k	Bias of the encoder of the DNN
$\widetilde{k}$	Bias of the decoder of the DNN
Q	Air flowrate, [m^3/s]
RMS	Root-mean-squared deviation
V_b	Bubble volume, [m^3]
X	Input vector of the DNN
$\hat{X}$	Estimation of X in the DNN pre-training
W	Weights of the encoder of the DNN in the pre-training
$\widetilde{W}$	Weights of the decoder of the DNN in the pre-training
μ_{slurry}	Dynamic viscosity of the slurry phase
μ_{fluid}	Dynamic viscosity of water
ρ_l	Water density, [kg/m^3]
ρ_{slurry}	Slurry density, [kg/m^3]
ρ_s	Solid density, [kg/m^3]
σ	Surface tension, [Nm]
φ_l	Water percent in the slurry phase
φ_s	Solids percent in the slurry phase
ϕ	Volume fraction of solids in the slurry phase

optimization strategy may be not effective when the gradient propagates across multiple nonlinearities. To avoid this limitation, in [7] it was presented a procedure which consists of pre-training one layer at a time, demonstrating that it is possible to learn in deep NN-architectures. In the recent years, the applications of this method with Restricted Boltzmann Machine have grown exponentially to address pattern recognition problems in computer vision [8], automatic speech recognition and natural language processing [9]. Surprisingly, despite the fact that DNNs have also been used for time series modeling and forecasting achieving promising results [10], the prediction problem has not been addressed exhaustively with DNNs.

2. Modeling CFD response with DNN

Reliable computational fluid dynamics (CFD) data are often used to simulate pressure and velocity fields in complex systems such as bubbly flows in different applications such as mineral froth flotation among others [11]. The CFD data and the uncertainties behind the use of turbulent frameworks collect features of realistic systems which may be validated with empirical and semi-empirical models [12,13]. In [14] experimental and CFD results of two-phase fluid flow in a tube were predicted using ordinary NN. Those results showed that the NN can predict with a reasonable accuracy the complex flow. In this study, the bubble size and bubble rate are obtained using a set of CFD data. The prediction considered employs the leave-one-out strategy where the whole dataset but one is used to train the DNN tool predicting the one not seen in the training step. This procedure is repeated by shifting the unseen data to the next one until completing the whole set of CFD data.

Fig. 1 shows the DNN architecture employed in this paper. In order to map both bubble size and bubble rate, two decoupled and independent DNNs are used. The first network is trained to learn the "hidden" function that estimates bubble size using the following inputs variables: initial velocity; fluid viscosity; fluid density; surface tension; and, contact angle. The second DNN is trained to learn the "hidden" function that outputs the bubble rate from the same set of inputs. It is worth highlighting that four out of the five input variables correspond to

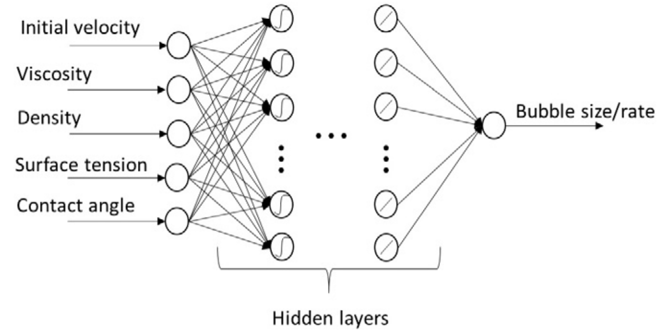

Fig. 1. The DNN architecture employed to learn the hidden function that delivers the bubble size and rate by making use of the following information: gas inlet velocity; fluid viscosity; fluid density; surface tension; and, contact angle.

fluid characteristics that are possible to be measured. The fifth input variable represents the inlet velocity computed with respect to the cross surface area of the nozzle throughout which the air injected into the simulated tank. The hidden layers activation functions are nonlinear (e.g. sigmoid), but the activation function of the output layer is linear. As a result of this procedure, the DNN architecture that is able to represent accurately the CFD results is reported.

3. Methodology

3.1. Details of CFD simulations

CFD simulations of bubbly flows were obtained from a 3D cylindrical system sketched in Fig. 2. It consists of a container 50 cm height and 20 cm diameter filled with fluid up to 40 cm. The gas flowrate enters at the bottom through an inlet located at the center of the base with a 2 mm diameter. A mesh of 600,122 cells was considered to resolve the mass balance and momentum equations according to the equations presented in a previous research work [15]. The fluid media considered in the research were pure water and slurry phase, where the latter is similar to that observed in mineral froth flotation operations, demonstrating the significant differences occurring when passing from a fluid free of solids and reagents (frother-free aqueous solution) to another with 30% solid with frother reducing its surface tension. The main properties of both fluids are presented as follows.

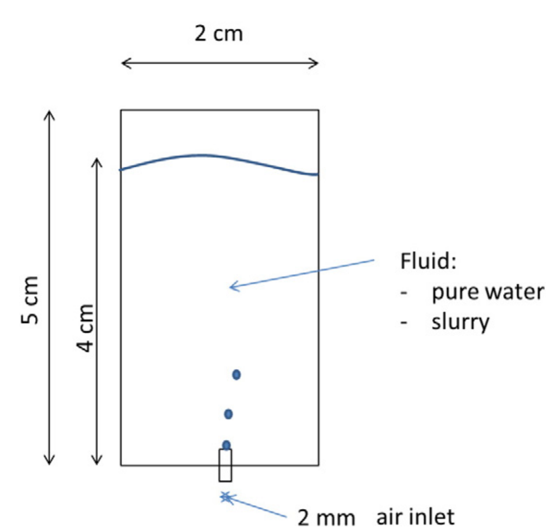

Fig. 2. Sketch of the CFD 3D cylindrical system used to obtain bubble volume and bubble rate.