CAMURE-11 11th International Symposium on Catalysis in Multiphase Reactors
ISMR-10 10th International Symposium on Multifunctional Reactors
MILANO, ITALY - 21-24 March, 2021

Gas-liquid flow regime prediction in microreactors by using dimensional analysis, regressions, and neuronal networks

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1. Introduction

The miniaturisation of process equipment is seen as a promising path to intensify chemical and biocatalytic reactions. Most of the processes involve several phases and in many cases gas and liquid. In the design of such microreactors for industrial applications, engineers need to know which flow regime is present inside the apparatus at applied conditions and for the employed feeds. Concentrating on gas-liquid flows and minichannels, most of researchers agree that there are six main flow regimes which are usually called annular flow, bubbly flow, churn flow, Taylor flow, Taylor-annular flow, and dispersed flow [1, 2]. The shift between these flow regimes is usually related to the gas and liquid superficial velocities and illustrated in flow regime maps. Parameters which affect the transitional velocities can be divided into a) material properties, such as surface tension, viscosity, and wall wetting properties, b) flow channel parameters, such as dimension, cross section, and flow orientation, and c) the applied inlet geometry. The literature provides several attempts to create flow regime maps which are based on dimensionless numbers. However, most of the published work used only selected data (mainly only one gas-liquid system), or are based on very limited experimental data, or use identical dimensionless numbers in the prediction of different regimes which is rather crucial because different forces, such as surface tension forces or inertial forces, dominate the flow in the different regimes and its development in the inlet section.

This paper employs the data of 27 publications in order to develop novel, universally applicable flow regime classifiers by two different methods.

2. Methods

By a systematic literature review, a database containing 97 flowmaps from 27 publications with 13156 data was built within this work. By using the Pi-theorem, 7 significant dimensionless groups were identified which dictate the flow regime transitions in microreactors, namely $u_{G,s}/u_{L,s}$, Re_G, Re_L, We_G, We_L, Θ^*, as well as a channel form factor $A_{Ch,q,cirmax}/A_{ch,q}$. The data of the data base were used to parametrise transition functions by nonlinear regression which describe the shifts between Taylor flow and the neighbouring regimes as well as to train neuronal networks which predict the different flow regimes. Both methods were implemented in MatLab®.

3. Results and discussion

By using nonlinear regression, the transition criteria of decision trees were developed which allow predicting whether there is Taylor flow in the channel. The criteria are basically mathematical functions describing the transition boundaries between Taylor and bubbly, Taylor-annular, or churn flow. It was found that these boundaries are significantly affected by the employed inlet design. In consequence, individual decision trees for T-, Y-, and cross-junctions, as well as static mixer geometries were developed to achieve a reasonable model accuracy (generally $R^2>0.93$).

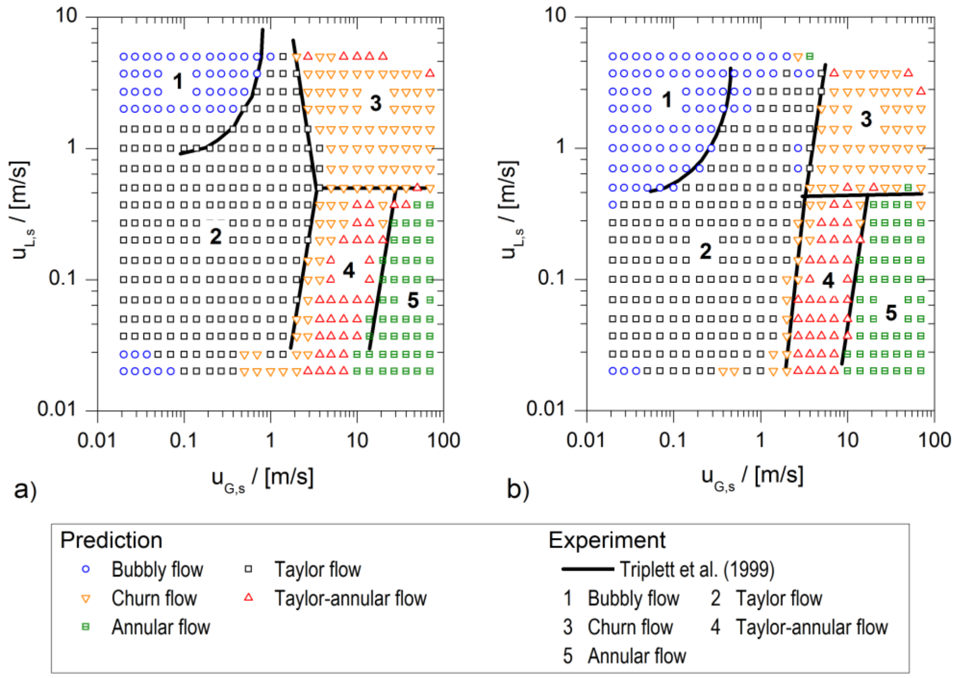

Figure 1. Comparison between flow regime predictions using the neuronal network trained with experimental data using cross-junctions and experimental observations by Triplett et al. [3] for a channel diameter of a) 1.097 mm and b) 1.45 mm.

In order to reduce the manual and analytical efforts in developing a complete flowmap containing 8 or even more boundaries, an artificial neuronal network classifier (ANN-classifier) was created which contains a feed-forward backpropagation network. As expected, different classifiers had to be developed by training the network exclusively with data of only one inlet designs to get reasonable results. By using these classifiers, flow regimes could be successfully discriminated (R=0.92...0.95 and classification rate was generally above 80%). It is recommended to use these classifiers to predict flow maps as illustrated in Fig. 1 instead of predicting the flow regime at specific conditions directly. By doing so, physical meaningless outliers can be easily detected, which significantly reduces model mismatching (about 50%).

4. Conclusions

Both methods provided reasonably precise flow regime classifiers. From the scientific point of view, trained ANN-classifiers allow fewer insights into the physics behind because they do not provide explicit rules, i.e. they operate more or less like a black box. However, the regression analysis in this work also resulted in complex interactions of the various dimensionless groups which are different for each inlet. This makes it also difficult to draw physical sound conclusions from the regression analysis. Furthermore, the creation of the ANN-classifiers by employing the neuronal network toolbox of MatLab® was straightforward and less time consuming.

References

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