Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Dynamic analysis for prediction of flow patterns in an oscillatory baffled reactor using machine learning

Hideyuki Matsumoto[a]*, Yuma Kambayashi[a], Shiro Yoshikawa[a], and Shinichi Ookawara[a,b]

[a] Institute of Science Tokyo, Department of Chemical Science and Engineering, Tokyo, Japan
[b] Yasuda Women's University, Department of Aesthetic Design and Technology, Hiroshima, Japan
* Corresponding Author: matsumoto@mct.isct.ac.jp

ABSTRACT

In the present paper, we come up with application of machine learning using data for flow visualization as a method for predicting unsteady flow patterns in oscillatory baffled reactors (OBRs). Application of the proper orthogonal decomposition (POD) is investigated for dynamic analysis of spatio-temporal data acquired by particle image velocimetry (PIV) to determine inputs and outputs for neural network model. It has demonstrated that three sets of modes and time-varying mode coefficients extracted by the POD could be useful for dynamic analysis and prediction of time-variant flow patterns in OBR. Also it is shown that decomposition of the time-series data for the mode coefficients by Fourier series expansion was effective for deriving reduced order model.

Keywords: Oscillatory baffled reactor, Proper orthogonal decomposition, Neural network model

INTRODUCTION

An oscillatory baffled reactor (OBR) [1] is a type of flow reactor, and is generally structured with equally spaced baffles arranged inside a circular tube. In this reactor, the fluids in the reactor are mixed by periodically oscillating the fluids or the baffles. Tubular reactors and continuous stirred tank reactors (CSTRs) have been widely used as conventional flow reactors. Tubular reactor is a type of reactor in which the fluids flow continuously in one direction with reaction, and has a simple structure. However, it requires a large flow rate to sufficiently promote the mixing of the fluids, which results in a problem of consuming a lot of power. In addition, for long tube reactors that are applicable to slow reaction, there are limitations for implementation in terms of installation space and cost. On the other hand, CSTRs have the advantage that the fluids are sufficiently mixed in each stirred tank, but in order to attain a uniform residence time distribution, a large number of stirred tanks must be connected in series, which causes the system to become complicated.

OBRs are attracting attention for their process intensification effects, such as high mixing performance at low flow rates and long residence time due to the vortices generated by the interaction between the oscillating flow and the baffles. Due to high performances for mixing and mass transfer, the OBRs are applied to various process systems. For example, for applications of OBRs to gas-liquid reactions, the reaction efficiency could be enhanced by increase in the contact area between the gas and liquid that is caused by oscillating flow. For liquid-liquid reactions, OBRs could be applied to achieve uniform mixing of two phase flow. Also, for application of OBRs to solid-liquid reactions, it has been observed that oscillating flow between baffles performs well-dispersion of solid particles, which leads to intensification of the reaction process. Due to the above-mentioned process intensification effects, OBRs are being put to practical use in various industrial fields, such as fine chemicals, pharmaceuticals and biodiesel productions [2-3].

In design of the oscillatory baffled reactors, optimal reactor performance could be achieved through complex interactions among multiple design parameters. The design parameters for OBR are related to geometry of baffle, structure of reactor and operation for generation of oscillating flow, so that they influence flow pattern inside reactor. The design of the flow in OBR is evaluated by several dimensionless numbers, including the oscillatory Reynolds number), the Strouhal number (St), the velocity ratio and so on.

The oscillatory Reynolds number (Reo) [1] is an index representing the mixing intensity inside the OBR, and is expressed by the following formula.

$$Re_o = \frac{2\pi f x_0 \rho d}{\mu} \quad (1)$$

where f is the frequency of oscillation, x_0 is the amplitude of oscillation, ρ is the density of the fluid, and μ is the viscosity of the fluid. When $Re_O \leq 250$, the flow is axially symmetric and is defined as laminar flow. In a case when $250 < Re_O < 2000$, the flow is in the transition region, and the flow where $Re_O \geq 2000$ is generally considered as turbulent. In our previous study for application of OBR to three-phase hydrogenation of 3-butyn-2-ol by using Pd/Al_2O_3 catalyst, OBR has demonstrated higher reaction performance than the conventional packed bed reactor (PBR), and at the same Re_O, OBR with lower amplitude attained higher conversion [4].

As shown Figure 1, it was considered that the difference in f and x_0 influenced the flow pattern inside the reactor and behavior of the reaction process (e.g. conversion X) for a case when frequency and amplitude differ with the same Re_O. As a result of flow visualization, since the generation of vortices was remarkably observed in the vicinity of the loaded catalyst when the amplitude x_0 was smaller, it was thought that analysis and prediction of the time-dependent changes in the local circulating flow in the region between the baffles would lead to more efficient design of OBR.

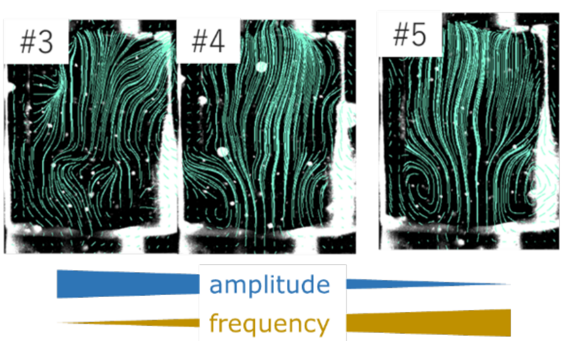

Figure 1. Comparison of streamlines that was obtained by PIV (#3: $x_0 = 15mm, X = 36.4\%$, #4: $x_0 = 10mm, X = 43.9\%$,#5: $x_0 = 5mm, X = 52.2\%$).

Although it is well known that computational fluid dynamics simulations [5-6] are effective in analysis and prediction of the flow patterns, there is a problem in that calculations for unsteady processes require a high computational load. Therefore, we came up with application of machine learning using data for flow visualization as a method for predicting unsteady flow patterns. In the present paper, we investigated methods for dynamic analysis of spatiotemporal data acquired by Particle Image Velocimetry (PIV) to determine inputs and outputs for neural network model.

METHODOLOGIES

Acquisition and analysis of flow visualization data

Figure 2 shows a schematic diagram of the oscillatory baffled reactor used in the flow visualization experiment using particle image velocimetry (PIV). The reactor is an acrylic tube type with an inner diameter of 26 mm. Baffles with a diameter of 25 mm and an opening area of 25% are placed in the reactor at equal intervals of 35 mm. The center part of the reactor tube with a length of 250 mm is covered by a rectangular vessel that is filled with water to eliminate distortion due to light refraction.

The flow rate of the steady flow was controlled by a plunger pump (FLOM, KP-22), and the oscillatory flow was generated from the bottom of the reactor using a syringe pump (Hamilton, PSD/6). Polyamide particles KP-050 (Kato Koken), which have a specific gravity almost the same as that of water, were used as tracer particles. The flow was visualized by irradiating the tracer particles with a green laser sheet formed by a PIV laser G2000 (Kato Koken). The motion of the tracer particles was recoded by using a high-speed camera (Kato Koken, k-8HD), and the obtained image data was analyzed by PIV software (Kato Koken, Flow Expert).

Table 1 shows operating conditions for acquisition of flow visualization data. Oscillatory Reynolds number Re_O, the flow rate of the steady flow Q, the amplitude of oscillation of syringe pump x_O, and the frequency of oscillation of syringe pump f were changed in the present experiments.

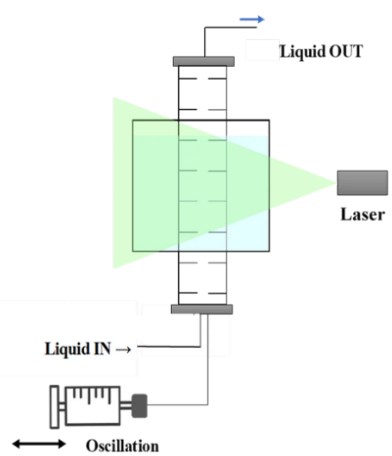

Figure 2. Schematic diagram of flow visualization experiment systems including OBR.

Table 1: Operating conditions for flow visualization experiments.

Re_O [-]	762, 595, 293, 142, 40
Q [ml/min]	8.3, 16.6
x_O [mm]	5, 10, 15
f [Hz]	0.02 – 1.06l

Application of the proper orthogonal decomposition (POD)

Recently, in the fields of computational fluid dynamics simulation, an approach that integrates the reduced order modeling (ROM) with machine learning technology has been investigated [7]. The major ROM techniques include the principal component analysis (PCA) and the proper orthogonal decomposition (POD) [8]. Application of the he ROM techniques can efficiently extract important information from phenomena by reducing the dimensionality of high-dimensional data, enabling accurate learning and highly accurate modeling of even highly nonlinear phenomena, enabling advanced prediction and analysis.

In the present paper, we investigate applicability of POD to reduced order modeling of spatiotemporal PIV data for OBRs. As mentioned above, POD is a modal decomposition method widely used in the field of fluid dynamics, which is used to efficiently reduce the dimensionality of huge amounts of data and extract the dominant structures in the flow field. POD is effective for analysis of unsteady flow, and is known as a method to clarify the essential characteristics of complex flow phenomena. POD calculates a spatially accommodating structure called "mode" based on a given data set, sorts the modes in order of contribution, and reduces the dimensionality of the data by selecting the dominant mode from the top.

In POD analysis, flow field data is decomposed based on the following formula.

$$\boldsymbol{q}(\boldsymbol{\xi},t)-\overline{\boldsymbol{q}}(\boldsymbol{\xi})=\sum_{j=1}^{r}a_j(t)\boldsymbol{\phi}_j(\boldsymbol{\xi}) \tag{2}$$

where $\boldsymbol{q}(\boldsymbol{\xi},t)$ is the time- and space-dependent flow field data, $\overline{\boldsymbol{q}}(\boldsymbol{\xi})$ is the time-averaged flow field data, $a_j(t)$ is the time-varying coefficient corresponding to each mode, $\boldsymbol{\phi}_j(\boldsymbol{\xi})$ is the spatial eigenmode, and r is the total number of modes. In this decomposition, the spatial modes $\boldsymbol{\phi}_j(\boldsymbol{\xi})$ are obtained by solving the eigenvalue problem of the covariance matrix.

$$\boldsymbol{R}\boldsymbol{\phi}_j=\lambda_j\boldsymbol{\phi}_j \tag{3}$$

where $\boldsymbol{R}$ is the covariance matrix, and λ_j is the eigenvalue indicating the contribution of each mode.

The covariance matrix $\boldsymbol{R}$ is defined as follows:

$$\boldsymbol{R}=\sum_{i=1}^{m}\boldsymbol{x}(\boldsymbol{t}_i)x^T(t_i) \tag{4}$$

The time-varying mode coefficients $a_j(t)$ represent the contribution of each POD mode at a particular time. The time-varying coefficients are calculated by the following equation:

$$a_j(t)=\langle\boldsymbol{q}(\boldsymbol{\xi},t)-\overline{\boldsymbol{q}}(\boldsymbol{\xi}),\boldsymbol{\phi}_j(\boldsymbol{\xi})\rangle \tag{5}$$

On the other hand, singular value decomposition (SVD) is sometimes used to calculate POD analysis, and is expressed as follows for a data matrix $\boldsymbol{X}$:

$$X=\boldsymbol{\phi}\Sigma\boldsymbol{\psi}^{\boldsymbol{T}} \tag{6}$$

where $\boldsymbol{X}$ is the data matrix, $\boldsymbol{\phi}$ is the left singular vector representing the spatial mode, Σ is the singular value representing the contribution, and $\boldsymbol{\psi}$ is the right singular vector representing the time-varing coefficient indicating the temporal change of each mode.

RESULTS AND DISCUSSION

POD analysis of PIV data for OBR

Figure 3 shows time variation of streamlines that were obtained by PIV analysis when Re_O was 762, Q was 8.3 mil/min, and x_O was 5 mm. It was observed that the flow pattern changes in this order: at the moment the oscillating flow became a push-out flow, vortices are generated on both sides of the lower part. The vortices then disappeared and the vertical flow occurred. At the moment when the flow became pull-out flow, vortices were generated on both sides of the upper part, and then the vertical flow was seen again. For the same oscillatory Reynolds number ($Re_O=762$), when x_O was 15 mm, it was seen that the vortices generated at the bottom and top moved up and down respectively, and the vortices remained. It was also observed that the axial symmetry of the flow was broken.

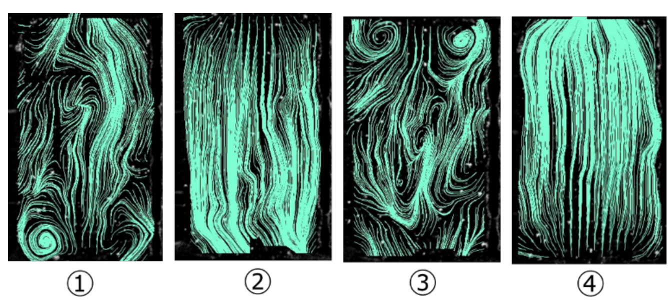

Figure 3. Time variation of streamlines that were obtained by PIV analysis.

As a result of POD analysis of the above-mentioned PIV data, the cumulative contribution of modes 1 to 3, which have the largest contribution, was about 80% (Figure 4). Figure 5 shows images of flow vectors that were reconstructed for three modes with the highest contribution which were selected from the more than 200 modes, for a case when Re_O was 762, Q was 8.3 mil/min, and x_O

was 5 mm. It was considered that the flow pattern for mode 1 represents profile of vertical flow and the flow pattern for mode 2 represents profile of generation of vortices in the upper and lower parts. Then Figure 6 plots change in calculated values of the time-varying mode coefficients $a_j(t)$. The trend in the time variation of $a_j(t)$ shows that POD could derive the reduced order model with characteristics of periodic changes in the flow pattern.

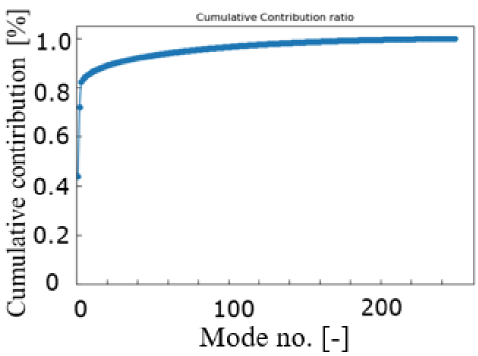

Figure 4. Variation of the cumulative contribution with increase in number of modes.

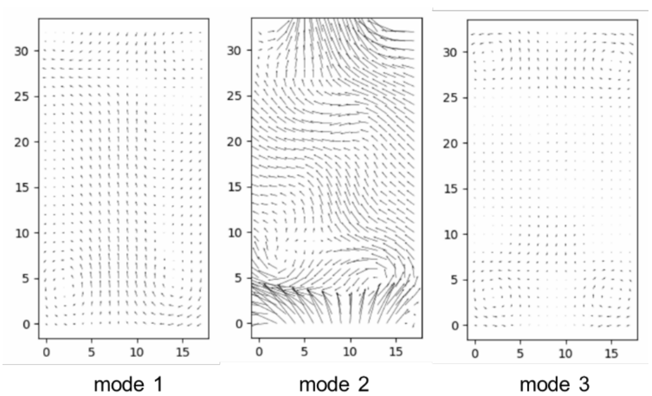

Figure 5 Images of flows of vector fields that were reconstructed for principal three modes.

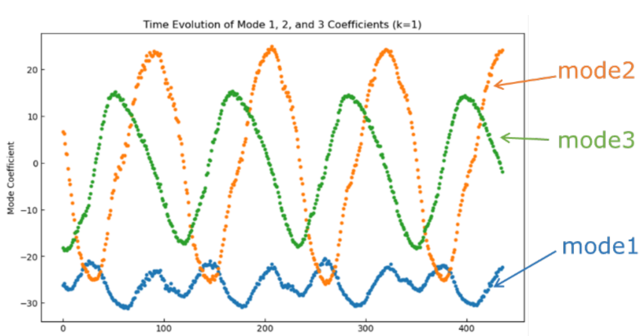

Figure 6 Time-series plots for time-varying mode coefficients.

Cases that the profile of vertical flow was extracted as mode 1 were seen when the amplitude x_O was larger. Even when the oscillatory Reynolds number Re_O was small and the flow rate of the steady flow Q was large, it was distinguished that the flows of vector fields for mode 1 showed profile of vertical flow. In addition, we analyzed the PIV data that were acquired by changing baffles with the different opening. When the baffle with small opening (16%) were used, it was experimentally observed position of generated vortices was upper part than cases of using the abovementioned baffles with 25% of opening. In application of POD analysis, the flows of vector fields with profile of generation of vortices in the upper and lower parts were extracted as mode 1, for case when the baffles with smaller opening.

Application of neural network modeling for prediction of flows of vector fields in OBR

We developed the multi-layered neural network model with three outputs of mode 1 – 3 that were extracted above, by using the no-code AI analysis platform "Multi-Sigma" (AIZOTH Inc.). In the modeling, oscillatory Reynolds number, amplitude and frequency of oscillation of syringe pump, velocity ratio for oscillatory flow and local velocity vectors were set as inputs. When training was implemented by changing the number of hidden layers from 1 to 10 and the number of hidden nodes from 3 to 96. As shown in Figure 7, results with high predictive performance were obtained for the generation, size, and movement of vortices. On the other hand, poor predictive performance was observed when Re_O was lower.

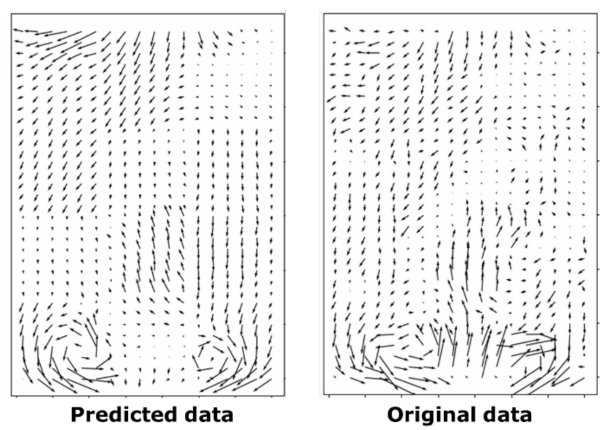

Figure 7 Recall of flows of vector fields by using the trained neural network model.

Next, methods for prediction of time-varying mode coefficients for the above mentioned three modes were investigated. In order to reduce dimensionality of data for the mode coefficients, we investigated application of decomposition of the time-series data for the mode coefficients into periodic integrals by Fourier series expansion:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_0\cos(nt) + b_n\sin(nt)) \quad (7)$$

Parameters $(a_0, a_1, \dots, a_n b_1, \dots, b_n)$ that were calculated by Eqs. (8) and (9) was used as outputs for multi-layered neural network model for prediction of the time-varying mode coefficients.

$$a_n = \frac{2}{T}\int_0^T f(t)\cos(nt)\,dt \tag{8}$$

$$b_n = \frac{2}{T}\int_0^T f(t)\sin(nt)\,dt \tag{9}$$

Combination of two types of neural network model for prediction of three mode (flows of vector fields) and for prediction of Fourier series expansion parameters related to the time-varying mode coefficients has demonstrated to show high predictive performance for time-varying streamlines in OBR.

While the proposed modeling approach has demonstrated the potential of black-box modeling for prediction of flow patterns, it was considered that the reliance on data-driven modeling without explicit physical insights may limit its generalizability across different reactor conditions. In future, it is necessary to focus on bridging machine learning models with first-principles approaches, ensuring a more interpretable and robust predictive framework for industrial OBR applications.

CONCLUSIONS

In the present paper, we investigated application of POD for dynamic analysis of spatio-temporal data acquired by PIV to determine inputs and outputs for neural network model. It was demonstrated that three sets of modes and time-varying mode coefficients extracted by the POD could be useful for dynamic analysis and prediction of time-variant flow patterns in OBR. Also it was shown that decomposition of the time-series data for the mode coefficients by Fourier series expansion was effective for deriving reduced order model.

In future, we will apply this proposed method to machine learning modeling based on CFD simulation data to clarify its superiority over CFD simulation. Furthermore, by clarifying the correlation between the feature quantities extracted from the CFD simulation data and the structural parameters of the reactor, it is expected that the I/O structure of a machine learning model could ensure a more interpretable and robust predictive performance for a wider range of reactor conditions.

ACKNOWLEDGEMENTS

This paper is based on results obtained from a project, JPNP19004, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

REFERENCES

1. Avila M., Kawas B., Fletcher D.F., Poux M., Xuereb C., Aubin J., Design, performance characterization and applications of continuous oscillatory baffled reactors. *Chem. Eng. Process.* 180: 108718 (2022)
2. McGlone T., Briggs N.E., Clark C.A., Brown C.J., Sefcik J., Florence A.J., Oscillatory Flow Reactors (OFRs) for Continuous Manufacturing and Crystallization. *Org. Process Res. Dev.* 19: 1186–1202 (2015)
3. Harvey A.P., Machley M.R. Seliger T., Process intensification of biodiesel production using a continuous oscillatory flow reactor. *J. Chem. Technol. Biot.* 78: 338–341 (2003)
4. Nabeshima M., Matsumoto H., Hamzah A.B., Yoshikawa S., Ookawara S., Analysis of Dynamic Behavior of Gas Bubbles and Solid Particles in an Oscillatory Baffled Reactor and Its Application to Design of Hydrogenation Processes. *Chem. Eng. Trans.* 94: 967-972 (2022)
5. Ni X., Jian H., Fitch A.W., Computational fluid dynamic modelling of flow patterns in an oscillatory baffled column. *Chem. Eng. Sci.* 57: 2849–2862 (2002)
6. Mazubert A., Fletcher D.F., Poux M., Aubin J., Hydrodynamics and mixing in continuous oscillatory flow reactors—Part I: Effect of baffle geometry. *Chem. Eng. Process.* 108: 78–92 (2016)
7. Shin J.H., Cho K.W, Comparative study on reduced models of unsteady aerodynamics using proper orthogonal decomposition and deep neural network. *J. Mech. Sci. Technol.* 36: 4491–4499 (2022)
8. Ooi C., Le Q.T., Dao M.H., Nguyen V.B., Nguyen H.H., Ba T., Modeling transient fluid simulations with proper orthogonal decomposition and machine learning. *Int. J. Numer. Meth. Fl.* 93: 396–410 (2021)