Validation of a DEM Modeling of Gas-Solid Fluidized Bed using the S-statistic in the State-Space Domain

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ABSTRACT
A reliable method was developed to validate results of a gas-solid bubble fluidized bed model with discrete element method (DEM) through comparison of corresponding pressure fluctuations experimental data. Attractors of two independent pressure signals, evaluation series of DEM model and reference time series of measured pressure signals, were compared in the state-space domain using the S-statistic. Comparison between two reconstructed attractors of evaluation and reference series was performed based on the null hypothesis. The null hypothesis that the evaluation and reference time series originate from the same dynamic sources is rejected if the two series significantly differ. To prove the power of the method, the S-statistic was estimated for obtained experimental data under the same operating conditions. In addition, experimental and model pressure fluctuations were decomposed into 9 levels using wavelet transform to study the validity of the model in a broad range of frequencies. Results indicated that the model results were consistent with experiments.

Keywords: S-statistic; Null-hypothesis; Discrete wavelet transform; Discrete element method (DEM); Fluidized bed

1. INTRODUCTION
In recent years, two main categories of CFD models such as two fluid models [1], discrete particle models [2, 3] have been conducted to study the hydrodynamic behavior of particulate flows. Among these models, DEM holds the greatest potential for long-term usefulness [4]. The increasing use of CFD codes as an engineering tool for predicting the flow behavior in many fields (e.g. multiphase flow (fluidized beds), earth sciences, management and operating research, physics, radioactive waste disposal, ship hydrodynamic [4]) is the main reason to devise new methods for comparison of signals. Although several aspects of comparison between CFD codes and experimental data were reviewed, these models have not been properly validated [4]. Van Wachem et al. [1] showed the agreement of a Two Fluid model (TFM) using dominant frequency and Kolmogrov entropy. Van Wachem et al. [2] validated three different implementations of the Lagrangian-Eulerian model by power spectral density function. Grace and Taghipour [4] proposed a series of recommendation for modelers who wish to test their modes against experimental data. Diks

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et al. [5] introduced the S-statistic based on a general distance concept between two delay vectors that provides a consistent test for the null hypothesis. They demonstrated that two sets of independent vectors were obtained from the same probability or not. In many applications of gas-solid fluidized beds, the hydrodynamics of the bed may change over time, either by imposed alterations, like a grade change, or by undesired phenomena, like agglomeration. In both cases, the S-statistic can be applied to detect changes in an early stage as was developed by van ommen et al. [6].

The present paper is not concerned with different modeling approach, solution techniques or challenges facing CFD models. The S-statistic was represented to answer the question of whether the model results show significant differences in the fluidized bed hydrodynamic in comparison with experiments, without giving information about the nature of the differences. Time series pressure fluctuations of the model were extracted from the work of Mansourpour et al. [2]. The comparison is based on a discriminating statistic computed for the model and experiment signals. The null hypothesis is rejected if the discriminating statistic of two signals is significantly different.

2. EXPERIMENTS

The experimental set up is schematically shown in Figure 1. Experiments were carried out in a gas-solid fluidized bed made of a Plexiglas-pipe of 15 cm inner diameter and 2 m in height. Air at ambient temperature entered the column through perforated plate distributor with 435 holes of 7 mm triangle pitch. Cyclone was used to separate air from particles at high superficial gas velocities. Pressure probe (model SEN-3248 (B075), Kobold Company) was screwed onto the gluing studs located at 5 above the distributor. Pressure fluctuations were recorded in approximately 164 sec corresponding to 16384 data. Sampling frequency was 100 Hz and pressure fluctuations were measured in a laboratory-scale fluidized bed which operated in bubbling regime. Polyethylene particles (Geldart B) with mean sizes of 600 μm and a particle density of 920 kg/m³ were used in the experiments. The minimum fluidization velocity \( U_{mf} \) was estimated to be 0.1 m/s based on Wen and Yu correlation [7]. Experiments and model were conducted at superficial gas velocity of 0.55 m/s. The time series of pressure measurement were recorded 6 times to demonstrate the method is able to identify the similar source of hydrodynamic at the same conditions.

3. METHOD OF ANALYSIS

3.1 ATTRACTOR RECONSTRUCTION

There are three domains to analysis pressure signals including time domain, frequency domain and state space. In this work, a combination of frequency domain (wavelet transform) and the state space (S-statistic) was applied to investigate the compatibility of the results of the DEM with experimental data in the bed. To compare the model results with the time series of pressure measurement, it is essential to first reconstruct a phase space attractor from each time series. Several methods have been applied to reconstruct an attractor [8]. The method of time delay was chosen in the present paper which is simple in use [8]. The state-space was reconstructed from a scalar time series by copying time delayed components of the original time series in the reconstructed state space. A sampled time series (e.g. pressure signals) \( x(i) \) with \( i=1,2,3,...,N \), can be transferred into a set of \( N-(d-1)\tau \) vectors \( s(i) \) in the state space as follows:

\[
S(i) = [x(i), x(i + \tau), \cdots, x(i + (d-1)\tau)]
\]  (1)
$\tau$ and $d$ (embedding parameters) are time delay and embedding dimension, respectively. The embedding parameters were determined based on methods addressed by Zarghami et al. [8]. Time delay was assumed to be one and embedding dimension was estimated using time window method [8]. Optimum value of embedding dimension was estimated as one-quarter of the dominant or average cycle time. Average cycle time is defined as:

$$T_c = \frac{\text{length of total time series (in time units)}}{\left(\text{number of crossing with the average of time series}\right) / 2}$$

(2)

3.2 THE S-STATISTIC

Reconstructed attractors from two independent time series were compared using a discriminating statistic which was proposed by Diks et al. [5] to reject or approve the null hypothesis. The experimental time series were referred to reference and DEM-CFD pressure fluctuations were considered as evaluation time series. The length of evaluation series was taken one-fifth of the length of reference series. The reference time series was divided into five segments and each of them was compared with the model time series. The difference was expressed as the S-statistic which is defined by Eqn.(3):
\[ S = \frac{\hat{Q}}{\sqrt{V_c(\hat{Q})}} \]  

The S value is a random variable with zero mean and standard deviation equal to unit according to the null hypothesis. The null hypothesis rejects when estimated value of S is larger than three with 95% confidence level which represents these two delay vector distributions do not originate from the same sources [6-7]. The S value helps compare two signals generally however it is unable itself to detect differences in different frequencies. Using the ability of Multi-resolution analysis (MRA) as an appropriate tool and the S-statistic, one gets to compare the model and experimental signals in a broad range of frequencies.

### 3.3 MULTI-RESOLUTION ANALYSIS (MRA)

Based on multi-resolution analysis developed by Mallet [9], Rioul and Duhamel [10], the time series of \( x(t) \) can be decomposed into various scales of orthogonal signal component. They are the approximation sub-signals \( A_j(t) \), detail sub-signals \( D_j(t) \) which represent the components of \( x(t) \) at different resolutions, as the following equations:

\[
A_j(t) = \sum_k a_{j,k} \Phi_{j,k}(t) \quad k = 1, 2, \ldots, N / 2^j, \quad j = 1, 2, \ldots, J
\]

\[
D_j(t) = \sum_k d_{j,k} \Psi_{j,k}(t) \quad k = 1, 2, \ldots, N / 2^j, \quad j = 1, 2, \ldots, J
\]

An appropriate choice of \( J \) (the maximum level of wavelet transform) is taken at a specific threshold value of Shannon entropy where its value equals to zero [11]. In fact, the essence of discrete wavelet transform is to expand a time series (e.g. \( x(t) \)) as a sum of base functions \( \Phi_{j,k}(t) \) and \( \Psi_{j,k}(t) \). The approximation sub-signals are high level (low frequency) components which can be calculated using a low-pass filter while the detail sub-signals are related to low-level (high frequency) [12]. The frequency band of approximation and detail sub-signals are given by:

\[
D_j(t) = \left[ 2^{-(j+1)f_s}, 2^{-(j)f_s} \right]
\]

\[
A_j(t) = \left[ 0, 2^{-(j+1)f_s} \right]
\]

Based on the orthogonality and the energy conservation of wavelet transform, the total energy of signal can be calculated by:

\[
E = \sum_t \|x(t)\|^2 = \sum_{j=1}^J E_j^D + E_j^A
\]

The normalized energy of \( A_j(t) \) and \( D_j(t) \) are calculated as follows:

\[
E_j^A = \frac{1}{E} \sum_{t=1}^N \|A_j(t)\|^2
\]

\[
E_j^D = \frac{1}{E} \sum_{t=1}^N \|D_j(t)\|^2
\]
By means of MRA, the pressure fluctuations of the model and experiment were divided into multi-scale signals called macro, mezzo and micro scales which describe the behavior of the original signal [13]. The micro scale is represented by the scale $D_1$, $D_2$ and $D_3$ (high frequency components) which is attributed to particle motions and particles interactions with each other and the wall bed. The mezzo scale, corresponding to small bubbles, voids and cluster is captured by $D_4$, $D_5$ and $D_6$. The macro-scale is related to large bubbles and low frequency components (the summation of $D_7$, $D_8$, $D_9$ and $A_9$ sub-signals) [13].

4. RESULT AND DISCUSSION

One of the measured time series at similar conditions was utilized as the reference time series to compare with five evaluation time series. The reference time series have a length of 150 sec. which was divided into five parts of 30 sec. For each of these partial time series, the S value was estimated by comparing with an evaluation time series of 30 sec. Figure 2 gives the S value as a function of the time duration of the reference time series based on the comparison of five sections of the reference time series with an evaluation time series. In every test, the evaluation time series was chosen from one of five measured signals. All the S-values calculated for different evaluation time series are less than three. It can be concluded that the null hypothesis (the similar hydrodynamic of two signals) cannot be rejected. Therefore, the method is able to be applied for the comparison between model and experimental results.

Figure 3 shows that the S-value calculated using the comparison of five parts of an experimental signal (reference time series) with the model signal against time duration of the experiment. The length of each segment of the reference and evaluation time series is 30 sec. The S-statistic is always below three through the reference time series. Therefore, the null hypothesis (i.e. similar hydrodynamic of experiment and model) cannot be rejected.
MRA was applied to investigate if model and experimental signals have the same dynamic or not in a wide range of frequencies. The decomposition level depends on the residual information on the sub-signals. The Shannon entropy of decomposed time series of pressure measured in the bed is illustrated at different level in Figure 4. The entropy of each approximate sub-signal decreases with increasing in decomposition levels. As can be seen in Figure 4, the Shannon entropy reaches to zero where the decomposition level is nine.
The energy distribution of MRA sub-signals is a useful tool to realize which sub-signal is dominant [13]. Figures 5a, b demonstrate the normalized energy distribution calculated from Eq.7 for the model and experimental sub-signals. As shown in Figures. 5a, b, the energy of detail sub-signals increases to reach a maximum value at $D_5$ and $D_4$ for the experiment and model sub-signals, respectively, then it starts to decrease. The highest energy among the sub-signals of model and experiment is observed in mezzo scale due to formation of small bubbles, clusters and voids. Therefore, mezzo scale is dominant scale based on the energy distribution of the model and experimental sub-signals.

In order to compare the sub-signals of the model and experiment in a broad range of frequencies, the S-value is estimated for three different scales according to Figure 6. The evaluation time series (model sub-signals) were compared to reference time series (experimental sub-signals) using the S-statistic through the reference time series. The obtained S-values from the comparison are less than three in more cases with the exception of mezzo scale. The S-value is more than three at three distinct points attributed to mezzo scale due to different hydrodynamic source. It shows that if the model signal is compared to five segments of experimental signal, the null hypothesis will reject for three segments corresponding to middle frequencies. In addition to this, the S values of dominant scale (mezzo) have the greatest values in comparison to other scales while the S value of micro scale is more than macro-scale. Therefore, the model can predict micro and macro scales better than mezzo scale and this is because the physics of the break-up of clusters is not properly captured in DEM. In general, it indicates that the main difference between the model and experiment is observed where the energy of sub-signals corresponding to different scales shows the maximum value. On the other hand, the null hypothesis was not rejected at high and low frequencies because of the same dynamic sources like noise in experiments and some errors in modeling (computer round-off errors, insufficient convergence of iterative procedure) at high frequencies and the existence of large bubbles at low frequencies. The S value of macro scale is less than micro scale which reveals that the results of DEM are more acceptable at low frequencies in comparison with high frequencies.
5. CONCLUSION

In this study, the pressure signals obtained from a DEM model and experiment were compared by the S-statistic. In general, the experimental and model results were in agreement. The pressure fluctuations of model and experiment were decomposed to nine levels corresponding to macro, mezzo and micro scales. The normalized energy of model and experiment showed that the mezzo scale is dominant scale in the experiment and model signals. Each scale of experiment and model was compared using the S-statistic. Except for some S values of mezzo scale, in other cases, the S value was less than three which indicated the same hydrodynamic source of the model and experiment.

NOMENCLATURE

- $a_{j,k}$: approximation coefficient
- $A_j$: approximation sub-signal
- $d$: embedding dimension
- $d_{j,k}$: detail coefficient
- $D_j$: detail sub-signal
- $E$: Total energy of signal, kPa$^2$
- $E^D_j$: energy of detail sub-signal, kPa$^2$
- $E^A_j$: energy of approximation sub-signal, kPa$^2$
- $f_s$: sampling frequency, Hz
- $i$: counter
- $J$: maximum decomposition level
- $N$: total number samples
- $\hat{Q}$: unbiased estimator of squared distance between two attractors
- $s$: state vector, point on state space attractor

Figure 6. The $S$- value of different scales
estimator for the normalized squared distance between two attractors

$t$ time, s

$T_C$ average cycle time, s

$U_{mf}$ minimum fluidization velocity, m/s

$V_c$ conditional variance

$x$ pressure fluctuation signal, kPa

GREEK SYMBOLS

$\Phi_{j,k}$ shifted function

$\tau$ time delay

$\Psi_{j,k}$ mother wavelet function

REFERENCES


