Simulation of adsorption processes in gas cleanup filters

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Abstract

New emerging technologies developed for efficient, clean, coal processing require research into the phenomena used in these processes. In this paper we will deal with the problem of cleaning gas obtained by means of coal gasification. Realisation of this process takes the form of filters with various properties. The efficiency of the gas cleaning process can be influenced by several factors. One class of factors is the physical properties of the granules used in the filter. These properties influence the way the granules move in the filter bed. Another class of problems concerns the adsorption properties of the granules. The quality of adsorption influences the efficiency of a filter and thus the costs of the gas cleaning process. The optimal combination of adsorption and physical properties of granules leads to the optimal exploitation of the filter, both from the point of view of costs and the degree of gas cleaning. While the physical properties of granules have been investigated, the adsorption properties still remain an unknown factor (or at least a factor with an unknown impact on the filter efficiency) from the point of view of filter design and exploitation. The main goal of our research was to investigate and simulate the adsorption capability of granules. The expected result was the determination of optimal counterplay between physical and adsorption processes. A simulation model with visualisation module has been developed and implemented.

1 Introduction

The development of devices based on new technologies can be considerably speeded-up by means of computer models. They are used for the simulation of the functionality of devices that are based on these new technologies. Such an approach leads to the acceleration of the design and consequently to the quick
production of such devices. When using computer models of devices (based on formal models of corresponding physical phenomena) it is possible to perform many more experiments than with real devices or real models of these devices. The intensive testing of the model leads to higher quality of final design. Moreover, it is possible to perform tests that can not be performed with real models due to the dangerous consequences of some tests that may lead to the destruction of the real model etc.

This paper deals with the design of gas cleanup filters that could be used for flue gas cleanup. We deal mainly with granular moving bed filters as this type of filters is one of the most promising approaches in the field of particle collection technologies in last years. The aim of our research is to investigate the behaviour of these filters in order to design effectively their configuration and mode of exploitation. Especially the second topic is of extreme importance. In the event of our being able to optimise the speed of movement of granules (using formal models - e.g. [1,2]), both in relation to the speed of the gas cleaned and the adsorption parameters of granules, we will significantly reduce the cost of the gas cleaning process.

The first step leading to a high quality device is the design of configuration of the filter. The optimum configuration prevents the existence of stagnant zones where granules accumulate and do not move either at all or with very small velocity. This results in poor efficiency of the exploitation of granules in the filter volume and to an increase of the pressure lost in the filter. This question has been discussed in our previous paper [2]. The method for the simulation of the behaviour of granules in the filter was designed and implemented. The simulation results were verified by means of experimental results obtained from tests on a real model of the filter (see Fig. 1). The left picture represents the results of real tests and the right one is the result of simulation in corresponding time scale.

Besides the optimum granule movement, the gas cleaning up process has also other dimension. The role of the granules in moving granular bed gas clean up
filters is to perform adsorption of particles from the gas cleaned. It is obvious that the adsorption ability of the granules influences significantly the course of the cleaning process. The next step in the development of efficient filter is the inclusion of adsorption into our model. This approach will allow us to experiment with the filter model by varying different parameters of the process as a whole. It will be possible to set individual parameters of the process in various contexts and in such a way it would be possible to optimise behaviour of the filter from various points of view.

2 Adsorption modelling

The model used for simulation of the movement of granules has been based on the partition of the filter volume into a finite set of volume elements. The elements have cubical form and are of the same size. This approach allowed us to deal uniformly with all elements in the filter volume, which simplified the computational process. The state of a volume element is given by several parameters, such as the number and positions of granules in the element. From the point of view of the adsorption process we are interested in the parameter characterising the concentration of pollutants that is assigned to each element. This concentration is modified stepwise during the gas movement through the filter due to particle adsorption. The gas flow is modelled as the transition of concentration of pollutants between individual volume elements. The change in concentration of pollutants is determined by the number of granules in the volume element and by their adsorption capability. The adsorption capability is given by the following formula (known as Dubinin linearised formula):

\[
X = \frac{W_0}{V_T} \cdot \exp \left( -B \left( \frac{T}{\beta} \right)^n \left( \log \frac{P_s}{p} \right)^n \right)
\]

\(p_s\) - saturated pressure of benzene vapour, \(p\) - partial pressure of benzene, \(T\) - temperature, \(W_0 (W_s)\) - maximum volume of the adsorption space, \(V_T\) - molar volume of the adsorbed pollutant, \(\beta\) - coefficient of affinity, \(B\) - constant characteristic for adsorbent, \(n\) - Dubinin exponent

In our initial model we considered only the horizontal direction of gas flow, which allows us to transport easily the value of gas pollution between individual volume elements. This transport (in the form of a change of concentration) is described by the following formula:
\[
\rho_x(t + \Delta t) = s \cdot \rho_{x-1}(t) + \frac{(1-s)}{x_c} \cdot \rho_x(t)
\]

\[s = v_g \cdot \Delta t\]

Where \(x_c\) is the x-component of the dimension of volume element, \(v_g\) is the speed of the gas flow, \(s\) is the trajectory through which the gas travels within one time step (\(s \leq x_c\)), \(\rho_x(t)\) is the pollutant concentration in the volume element positioned at \(x\) co-ordinate.

### 2.1 Implementation and course of computation

The computation (and corresponding implementation) has been based on equations described above. The first step is initialisation of key variables that will be handled as constants for each particular case (\(V_T, B, T, \beta, \rho_s, W_o\)). The calculation of adsorption isotherm is rather demanding computationally. In our implementation we speeded up the calculation by pre-calculation of several values using the information about maximum pollution. By means of linear interpolation it is possible to acquire the necessary values.

The level of adsorption in one volume element is given (besides other factors) by the degree of filling of the volume element. It is necessary to calculate the share of each granule that is contained (mostly partially) in a volume element. It is obvious that the share of granule volume that is contained in volume element will be dependent on the distance of the centre of the granule from the centre of the volume element. The corresponding function has the following shape: see Fig.2.

![Diagram](image)

**Estimation of granule volume [%]**

**Distance from the centre of the volume element**

**u - 1/2 of the cube diagonal of the volume element**

**r - radius of the granule**

Fig.2 Function for calculation of the filling the volume element

In the event of more granules influencing the volume element, the given function has been used to calculate the information about the space occupied by granules.
in the volume element. According to equations that have been discussed earlier the adsorption has been calculated. The new concentration of pollutants in flue gas should be calculated and this concentration is transported to the next volume element (in a horizontal direction). The described calculation should be performed for all volume elements. This calculation represents one time step. The level of concentration of pollutants is different in various parts of the filter. A colour is assigned to each level of this concentration. In this way it is possible to visualise the situation in the filter during the gas clean up process.

This approach has been tested by means of a series of tests in which various shapes of filters have shown various capabilities of adsorbing particles from the gas. Initial experiments assumed that the gas passes through the whole cross section of the filter. In more realistic simulations there will be certain numbers of inlets and outlets through which the gas will flow. Moreover, it is possible to work with a more general model as shown in the next section of this paper.

3 Model extension

In reality there are several inlets and outlets through which the gas flows. Such a case is shown in Fig.3. It is possible to see that the adsorption capability of granules is soon exhausted in cases where the speed of gas flow is higher than a certain limit.

The next step is the investigation of situations when the inlets and outlets are mutually shifted in a vertical direction. This means that the optimal trajectory the gas flows is not horizontal (see Fig.3). As the basic assumption for our initial model was the horizontal gas flow, it is necessary to modify the model to our needs. This will be achieved by means of interpolation of the line segment with a certain slope, which will result in a sequence of horizontal and vertical short line segments. This approach is well known in computer graphics under the denotation Bresenham algorithm. This means that in points where the vertical segment occurs the information about pollution density is not transferred horizontally but vertically to the beginning of the following horizontal segment. From the new position the calculation continues in the same (horizontal) way. The results of these simulations can be seen in Fig.3.

Parameters of the simulation depicted in the Fig.3:

Gas passing through the filter:
- Angle of gas flow: 15°
- Speed of gas flow: 1m/s
- Level of pollution: 0.2 g/m³

Granules:
- Radius of granules: 5 mm
- Adsorption capability: $W=0.191 \times 10^{-3}$
It is possible to see from the figure above that the gas cleaning process is stabilised after 13 seconds. Then the pattern representing the course of gas cleaning process is stable and does not change. In order to get a better idea about the development of the gas cleaning pattern, several representative examples were magnified and presented in the lower part of the figure. The distribution of the pollution in various parts of the filter during the gas cleaning process gives a
very good idea about the course of this process. Below there are given examples of the gas cleaning process under different circumstances.

Figure 4 shows the situation for three different gas flow speeds (Test #1) with the same speed of movement of granules. For another speed of granules movement it would be possible to change the speed limit for adsorption capability exhaustion. In this case several inlets and outlets in horizontal configuration have been used. The remaining two tests show the influence of the louvers angle on the course of the gas cleaning process and to the exhaustion of adsorption capability of granules. The angle influences the number of granules used in the gas cleaning process and in such a way the adsorption capability of granules can be soon exhausted.

TEST 1# (louvers angle = 0°)

\[ v_x = 0.1 \text{ m/s} \quad v_x = 0.5 \text{ m/s} \quad v_x = 1 \text{ m/s} \]

TEST 2# (louvers angle = 0°)

\[ v_x = 0.1 \text{ m/s} \quad v_x = 0.5 \text{ m/s} \quad v_x = 1 \text{ m/s} \]
Fig. 4 Simulation of the gas cleaning under various conditions

According to the physical properties of the granules flow and the filter design it is possible to find an optimal exploitation of the granules by means of a combination of the number of the gas inlets and outlets and the flow gas speed. Fig. 4 shows that with a low speed of the gas flow the exploitation of adsorption capability of granules is low (Test #1 – Test #3: the case when the gas flow speed is 0,2 m/s). Having more vertical inputs and outputs the gas is not sufficiently cleaned (Test #1 – speed 0,5 and 1,0 m/s). A combination of
appropriate angle and speed of the gas flow (Test #3 – speed 0.5 and 1.0 m/s respectively) would allow us to obtain high purity of the gas cleaned. Also the degree of exploitation of granules will increase significantly.

4 Theoretical framework

The adsorption process can be described by means of the Dubinin equation mentioned above. It was necessary to investigate whether the theoretical assumptions correspond with the practical requirements of our application (moving granular bed gas cleanup filter). We performed practical experiments with the adsorption capabilities of charcoal. The aim of our experiments was to verify the shape of adsorption isotherms for the adsorption of benzene in charcoal. Charcoal and benzene are widely used as reference materials for this type of tests. The main attention has been paid to values of the Dubinin exponent within limits from 1 to 2 in order to acquire the best linear dependence. The results obtained show very good match between theory and experimental results [3] and [4] – see Fig.5.

![Figure 5: Validity test of linearised Dubinin equation](image)

The lines in the figure correspond to the calculations based on the Dubinin equation. The markers correspond to values obtained by means of the experiments mentioned above. This good match justifies the application of the theoretical model for the simulation of adsorption processes.

5 Conclusion and future work

The system designed and implemented makes it possible to investigate very deeply the behaviour of filters of a specific type. The main contribution of this
work is the possibility of performing a large number of experiments within a short period of time. The main target was simulation of the absorption capability of filters under various conditions. This parameter of the filter is influenced both by the speed the granules flow in the filter and by the degree of saturation of active granules. Another important parameter is the number of active input and output louvers. Their number considerably influences the course of the gas cleaning process. The parameter that should be carefully investigated in further studies is the angle under which the gas moves within the filter.

From these experiments it is easy to determine an optimum set up of filter parameters during filter exploitation. The data acquired from these simulations will allow to use these filters in an efficient way with a high degree of filtering effect with minimal costs. The results of simulations have very good match with the behaviour of real filters of the type used [5]. In such a way the practical applicability of the model has been proved.

Further research will deal with establishing the methodology that would allow the user to find optimum settings under various conditions of filter exploitation (like filter configuration, speed of gas flow etc.) and the chemical and physical properties of granules.

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