

CFD MODELLING OF PRESSURE DROP AND FLOW DISTRIBUTION IN PACKED BED FILTERS

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ABSTRACT

A CFD technique for predicting the performance of axisymmetric packed bed filters has been developed.

The effect on the pressure drop of a non-uniform voidage distribution within the filter bed has been modelled. A radial voidage distribution was derived from a predictive model based on a modified Mueller equation. The pressure loss through the bed was calculated from the Ergun equation, using the local voidage.

The technique has been validated against experimental measurements of pressure drop and velocity distribution in a model of a filter system for a range of filter parameters and inlet velocities. Generally good agreement has been obtained between experiment and predictions.

A model of vapour adsorption within the filter is currently under development.

1 INTRODUCTION

Packed bed filters have been used for some time to remove toxic gases and vapours from contaminated airstreams. DERA Porton Down, in conjunction with S&C Thermofluids Ltd, are currently developing a CFD technique for predicting the flow through filters of this type. The work so far has included experimental measurements of velocities and pressure drops through packed beds and accompanying CFD predictions of the flowfield using the PHOENICS code.

Earlier work carried out by DERA involved the development of a CFD model including a pressure drop formulation based on the Ergun equation [1], but using a uniform voidage for the filter bed. The predicted pressure drops appeared to show some level of agreement with measured values but indicated that further experimental data was required.

Further experimental work was then carried out by DERA in two areas. Firstly, further measurements of the velocity distributions and pressure drops were made, and secondly measurements were made of the voidage distribution within the packed beds. As a result, DERA have determined a formula for predicting the radial voidage distribution within a packed bed for a given filter diameter and bead size. A brief summary of this work is included below.

S&C Thermofluids were then asked by DERA to include the predicted voidage distribution in a CFD model of the filter bed, and to validate the CFD model in the first instance against pressure drop data for one bead size and filter geometry at various air velocities. Further validation was subsequently carried out for a range of filter configurations. The following paragraphs describe this work and present some of the results of the validation.

The initial CFD results showed reasonable agreement with the test data, but there remained some discrepancies between the measured and predicted velocity profiles [2]. It was felt that these discrepancies were possibly due to the turbulence model, or to axial variations in the measured voidage distributions which were not included in the model. Furthermore, no systematic study of the effects of grid dependence had been carried out. These areas have now also been examined [3], and the amendments to the model and new results are described below.

It is intended that the software will also be used for modelling chemical adsorption processes within the filter bed, in order to predict breakthrough characteristics – ie the point at which the filter can no longer absorb all the vapour contaminant being drawn

through it. An adsorption model is currently being developed - this model and some preliminary results from it are described below.

2 MODEL DESCRIPTION

2.1 Prediction of voidage distribution

The characteristics of the flow through packed beds are important in filter design and an understanding of the relationship between void fraction and flow distribution is essential. It has been shown, eg [4], that for flow through a fixed bed of uniform particles that there is a peak velocity approximately one particle diameter from the outer wall of the bed, which decreases sharply towards the wall and more gradually away from it. The fraction of the bed influenced by this velocity profile depends on the ratio of particle size to bed diameter.

The investigation of the radial voidage distribution of uniform spheres in cylindrical filter beds involved both studying available published data and image analysis of thin slices through beds of snowstorm packed spherical beads. In both cases the voidage is found to be a minimum about half a particle diameter from the wall of the bed, and then follows a damped oscillatory function until it reaches a constant value about 5 particle diameters from the wall, where the packing is random. Some measurements were also made of the axial variation in voidage along the bed centreline: at the ends of the bed this was of a similar form to the radial variation near the wall.

An empirical correlation for the radial voidage distribution was determined, based on a modified version of that proposed by Mueller [5].

$$\varepsilon = \varepsilon_b + (1 - \varepsilon_b)e^{-br}J_0(ar^*) \quad \text{for } 2.02 \leq d_b/d_p \quad (1)$$

where:

$$a = 8 - 3.15/(d_b/d_p) \quad \text{for } 2.02 \leq d_b/d_p \leq 13.0 \quad (1a)$$

$$a = 8 - 11.25/(d_b/d_p) \quad \text{for } 13.0 \leq d_b/d_p \quad (1b)$$

$$b = 0.315 - 0.725/(d_b/d_p) \quad (1c)$$

$$\varepsilon_b = 0.334 + 0.220/(d_b/d_p) \quad (1d)$$

$$r^* = r/d_p \quad (1e)$$

and J_0 is a zero order Bessel function of the first kind.

Voidage distributions for 2, 3 and 4 mm spherical beads in a 98mm diameter bed were calculated from this correlation for input to the CFD model described below. Figure 1 shows a typical radial voidage distribution.

2.2 Experimental modelling

Experimental measurements of pressure drop and velocity were made using a filter bed which was snowstorm packed with spherical beads of uniform size.

Air was drawn through the filter bed by a fan at the downstream end of the system. The pressure drop measured was for the whole filter installation including the inlet and outlet cones, as shown in figure 2. The inlet pipe extended a further 85cm upstream of the inlet pressure transducer.

The axial velocity was measured at stations 5mm apart radially across the bed, at positions 15mm upstream and downstream of the bed. Measurements were made over a range of inlet velocities for three filters consisting of 2, 3 and 4mm beads respectively, and for three inlet/outlet cone lengths – 20, 50 and 200mm. The inlet velocity was measured on the centreline just upstream of the inlet pressure transducer.

2.3 CFD model

2.3.1 Geometry and governing equations

A CFD model of the filter bed was set up which enabled a radially varying voidage distribution to be prescribed. The geometry modelled is shown on figure 2: the CFD model included a section of the inlet pipe from the pressure transducer location, the diffuser cone upstream of the bed, the bed itself and a similar section downstream as far as the downstream pressure transducer location.

The PHOENICS CFD code [6] was employed to solve the conservation equations for mass and momentum (the Navier-Stokes equations). The model took advantage of the axisymmetry of the geometry, so only radial and axial momentum equations were solved.

The radial mesh distribution was determined directly from the voidage distribution output from DERA's modified Mueller equation model. A mesh node was created for each data point in the distribution. The mesh distribution could therefore be controlled by the number and location of data points output from the voidage model. The axial mesh distribution was prescribed separately.

The air flowing through the system was assumed to be an ideal gas, with the density calculated from the local pressure and ambient temperature.

2.3.2 Turbulence modelling and boundary conditions

The Reynolds' number at the inlet varied from about 3000 to 25000 for the range of flowrates studied, so the flow in the region upstream and downstream of the bed was assumed to be turbulent. The standard, two-equation $k-\epsilon$ turbulence model [7] was used initially, with turbulence in the bed itself suppressed. Various modifications to this model

were investigated [3] in an attempt to improve the prediction of the velocity distribution, and the two-layer model of Rodi [8] (a low-Reynolds' number model which uses a prescribed length scale in the near wall region) was determined to be the most appropriate.

At the inlet to the CFD domain, the pressure and temperature were defined. A radial velocity distribution based on Nikuradse's log-law profile for fully developed pipe flow [9] was also specified - this was thought to represent the likely velocity profile in the system at this point better than a uniform velocity. Profiles for K and E were also specified, having been derived from published data for pipe flows [10].

At the downstream boundary of the domain, a mass efflux was specified, equivalent to:

(mean inlet velocity * inlet density * inlet area).

A no-slip condition was imposed at the pipe wall along the length of the domain, with the skin friction derived from a log law when the standard k- ϵ model was used.

2.3.3 Pressure loss source terms

In the region of the mesh where the bed was located, the voidage distribution was modelled by setting the volumetric porosity of the cells in the CFD model to the local void fraction as determined by equation 1. Since the locations in the voidage distribution output from the modified Mueller model were used to define the cell boundaries, and since the porosities are defined as piecewise constant across each cell, an average of two values is used to define the cell porosity.

A source term was included in the axial momentum equation to represent the pressure drop through the bed. This was calculated from the Ergun equation [1], which gives the pressure drop per unit length through a packed bed as:

$$\Delta p/L = 5 S_o^2(1-\epsilon)^2 \mu U/\epsilon^3 + 0.29 S_o(1-\epsilon)\rho U^2/\epsilon^3 \quad (2)$$

where ϵ is the local void fraction determined from equation 1 and U the superficial velocity (the velocity which would the fluid would have if no reduction in cross sectional area occurred). At any point in the bed, the superficial velocity is related to the interstitial velocity, u, calculated by the CFD code by $U = u.\epsilon$.

2.3.4 Adsorption model

A simple adsorption model has been set up within PHOENICS to demonstrate how the filtration process could be modelled. The model has been run transiently to demonstrate gradual saturation of the filter, and the effect on breakthrough of the non-uniform voidage distribution near the walls.

In the model a transport equation for the vapour concentration was solved in addition to the mass flow and momentum equations. An inlet concentration was derived from a nominal relative humidity and the ambient temperature.

Adsorption into the filter bed is modelled via a source term for the adsorption rate where the adsorption rate per unit fluid volume is:

$$-\partial C/\partial t = 1/\varepsilon S_o k (C - C_i) \quad (3)$$

A linearised version of this source term was included in the finite volume equation for the vapour concentration.

The rate of uptake of vapour in the adsorbent was calculated as:

$$\partial m/\partial t = \varepsilon/(1-\varepsilon) (-\partial C/\partial t) 1/\rho_z \quad (4)$$

and the cumulative uptake, $\Sigma (\partial m/\partial t \cdot \delta t)$, was stored for each cell in the bed.

For the results shown below the interfacial concentration, C_i , was assumed to be zero for any cell in the bed until the cumulative uptake for that cell exceeded the maximum value given by the isotherm equation. At that point, the adsorption rate was set to zero for that cell. Recent developments to the model include basing this interfacial value on an assumed local equilibrium between vapour and adsorbed fluid. This results in an adsorption rate which automatically falls to zero as the uptake reaches the maximum value.

The mass transfer coefficient, k , was derived from the Carberry correlation [11] which gives the Sherwood number for mass transfer in a packed bed as a function of the Reynolds' and Schmidt numbers.

The heat of adsorption of the vapour was not taken into account in the present model.

The local concentration of vapour was assumed to have a negligible effect on the thermodynamic properties of the air, and hence no effect on the predicted flowfield. This assumption enabled the steady-state flowfield solution to be 'frozen' during the transient run, so that only the vapour concentration equation was actually solved. This technique substantially reduced the CPU-time required for the transient runs.

2.3.5 Implementation of the model in PHOENICS

The radial voidage distribution for any given ratio of particle size and bed diameter was calculated using a spreadsheet package (MS Excel). This was then saved as a text file.

A FORTRAN program has been written to interpret the voidage distribution and other input parameters defining the model and to write out a Q1 file complete with grid generation

commands for the steady-state flow prediction. A supplementary Q1 file has been written for the additional commands required to run the transient adsorption model.

GROUND coding was also written in order to set the porosity in the filter bed from the voidage distribution, to calculate the pressure drop source terms and to set the inlet boundary conditions. The adsorption model source terms were also set via GROUND coding and additional subroutines were called from GROUND to access a database of vapour pressure and adsorbent isotherm data.

The model was initially developed for PHOENICS version 2.1 and later transferred to PHOENICS version 3.1. After some initial problems with the turbulence model in v3.1, both version gave similar, but not identical, results.

On a Pentium II PC, run times for the steady state flow prediction were of the order of 20 – 30 minutes and for the transient adsorption model 1 – 2 hours depending on the number of time-steps used.

3 RESULTS OF FLOWFIELD PREDICTIONS

3.1 Pressure drop

Initial results predicted by the CFD model, for a bed of 3mm beads and an inlet diffuser length of 200mm showed reasonable agreement with measured pressure drops over a range of velocities, especially when compared to predictions using a uniform voidage in the filter bed – see figure 3.

Comparison of predicted and measured pressure drops for 4mm beads also showed good agreement, but for 2mm beads there was a larger discrepancy between the CFD and experimental data. This discrepancy was significantly reduced by doubling the grid density in the radial direction to 150 cells (see figure 4). Refining the grid also improved the predicted pressure drop for the 3mm beads, but had little effect on the predictions for the 4mm beads where the grid size was already small compared to the bead size.

Changing the length of the inlet and outlet cones had little effect on the predicted pressure drop, a trend also apparent in the experimental data.

3.2 Velocity distribution

Initial predictions of the velocity distribution also showed reasonable overall agreement with experimental data. Upstream of the bed the maximum velocity was on the centreline, and downstream of the bed the velocity was higher towards the wall. However the radial variation was greater in the CFD predictions, and the velocity gradient downstream of the bed near the wall was much higher than that measured.

For the shorter cones (5 and 2cm) the discrepancy between CFD and experimental profiles upstream of the bed was even greater, with the CFD model predicting a separated region close to the wall which was not observed in practice. Various modifications to the CFD model were investigated to try to improve these predictions, including changes to the turbulence model, better representation of the geometry at entry to the inlet cone and accounting for any axial variation in voidage.

Increasing the voidage in the first and last cells in the bed in an attempt to account for the observed variation in axial voidage distribution within the bed had a small but adverse effect on the predicted velocity distribution. Clearly this characteristic cannot be adequately modelled by such a simplistic approach.

In the experimental rig there was a small radius at the junction of the inlet pipe and inlet cone. Smoothing the entry to the inlet cone in the CFD model produced a small improvement in the predicted velocity profile upstream of the bed for the 2cm cone (see figure 8), but had little effect with the longer cones.

Various modifications to the standard $k-\varepsilon$ turbulence model were investigated. Other high Reynolds' number two-equation models, viz. the RNG [12] and Chen-Kim [13] models, produced little if any improvement in the predicted velocity distributions. However inspection of the boundary layer along the wall of the system showed that values of y^+ in the near wall cells were of the order of 1, suggesting that the use of a high Reynolds' number turbulence model with standard log-law wall functions was inappropriate. Using a low-Reynolds' number model – the two-layer model of Rodi [8] – in conjunction with a finer radial grid distribution (as per figure 4) produced a marked improvement in the predicted profiles both upstream and downstream of the bed.

In order to obtain a converged solution with this turbulence model it was necessary to reinstate the generation terms for K within the bed, which had been suppressed when using the $k-\varepsilon$ model. This resulted in a small but acceptable increase (~3%) in the predicted pressure drop.

Figure 5 shows measured and predicted velocity profiles up- and downstream of a bed of 3mm beads with a 20cm inlet cone. Profiles are plotted for a mesh density of 150 cells in the radial direction for both the standard $k-\varepsilon$ and two-layer models. Figures 6 and 7 show the same results for the 5 and 2cm inlet cones. In addition, figure 7 shows the upstream velocity profile for the two-layer model in conjunction with a radiused entry to the 2cm inlet cone. All measured and predicted velocity profiles presented here were for an inlet centreline velocity of 4 m/s.

4 TRANSIENT PREDICTION OF ADSORPTION RATES

4.1 Existing model

Initially, data on the adsorption of water vapour by a 13X zeolite molecular sieve was used to test the adsorption model. The zeolite molecular sieve has been shown experimentally to have a voidage distribution that is approximated by a packed bed of 4mm spheres. In order to model the adsorption process, the pressure and flowfield predicted by the filter model for 4mm beads, 20cm cones and a mean inlet velocity of 4m/s were used as the initial conditions. The initial concentration of water vapour in the domain was zero.

At the inflow boundary the water vapour concentration was set to a value equivalent to 50% relative humidity. The zeolite density was estimated from the bed density, 700 kg/m³, and a mean voidage of 39.6%. The maximum uptake of water in zeolite for a particular humidity level is given by a Langmuir isotherm of the form:

$$m_{\max} = a.b.RH / (1 + b.RH) \quad (5)$$

where a and b are empirically determined constants.

Figure 8 shows the predicted water uptake (in g/g) at various times. The penetration of the water into the filter bed, and the subsequent breakthrough occurring at the wall can be clearly seen. Time steps of the order of 1s were used in this prediction.

These results are qualitatively similar to experimental observation, but the breakthrough times are longer than those measured in real filters. Also, in the model the vapour front remains very sharp as it moves through the filter bed, whereas in practice it tends to be more diffuse. Some attempt to address this shortcoming has been made by modifications to the existing source term described in section 2. The effect of these changes is currently being validated against measurements from a range of filter sizes and vapour/adsorbent combinations.

4.2 Future developments

The adsorption source terms currently used in the model are based on the assumption that the vapour diffusion from the bulk fluid to the particle surface is the controlling step in the adsorption process. However the adsorption rate will also be influenced by surface diffusion and the properties of the adsorbent [14]. Further research needs to be carried out to quantify these effects and to account for them within the CFD model. It may also be appropriate to take into account the phase change and heat of adsorption at this stage.

The marked difference in breakthrough time near the filter wall compared with that at the centre of the bed suggest that the filter performance is closely linked to the velocity

distribution in the bed, and hence the validity of any CFD predictions is dependent on the turbulence modelling. Further experimental validation of adsorption model may be useful in determining whether the treatment of turbulence within the bed is adequate in the current model.

5 CONCLUSIONS

A method for predicting the pressure loss and velocity distribution in packed bed filters has been developed. The method has been validated over a wide range of flow parameters for axisymmetric geometries.

The method has been implemented within the user-routines of a commercial CFD package (PHOENICS). A model of vapour adsorption has also been developed and implemented.

Areas to be addressed in any further work may include inclusion of the axial voidage variation, turbulence modelling within the bed and further development and validation of the adsorption model. Additionally, the data input procedure could be enhanced through the development of a simple menu interface and linking the voidage calculation to the rest of the input procedure.

6 NOMENCLATURE

C	vapour concentration, kg/m ³
C _i	interfacial vapour concentration, kg/m ³
d _p	bead diameter, m
d _b	bed diameter, m
D	diffusivity of vapour in air, m ² /s
k	mass transfer coefficient, m/s
K	turbulence kinetic energy, m ² /s ²
m	uptake of vapour, g/g
r	radial position in bed, m
RH	relative humidity (%)
S _o	bead specific surface, /m (=6/d _p for sphere)
u	local, or interstitial, velocity, m/s
U	superficial velocity, m/s (= u.ε)
u _τ	friction velocity, m/s (= (τ _w /ρ) ^{0.5})
y	distance from wall, m
y+	non-dimensional distance from wall (= y.u _τ /ν)

ν	kinematic viscosity, m ² /s
τ_w	wall shear stress, Pa
ρ_z	adsorbent density, kg/m ³
ε	local void fraction
E	dissipation of turbulence kinetic energy, m ² /s ³
$\partial C/\partial t$	adsorption rate per unit fluid volume, kg/m ³ /s
$\partial m/\partial t$	uptake rate per unit adsorbent mass, g/g/s
δt	timestep size, s

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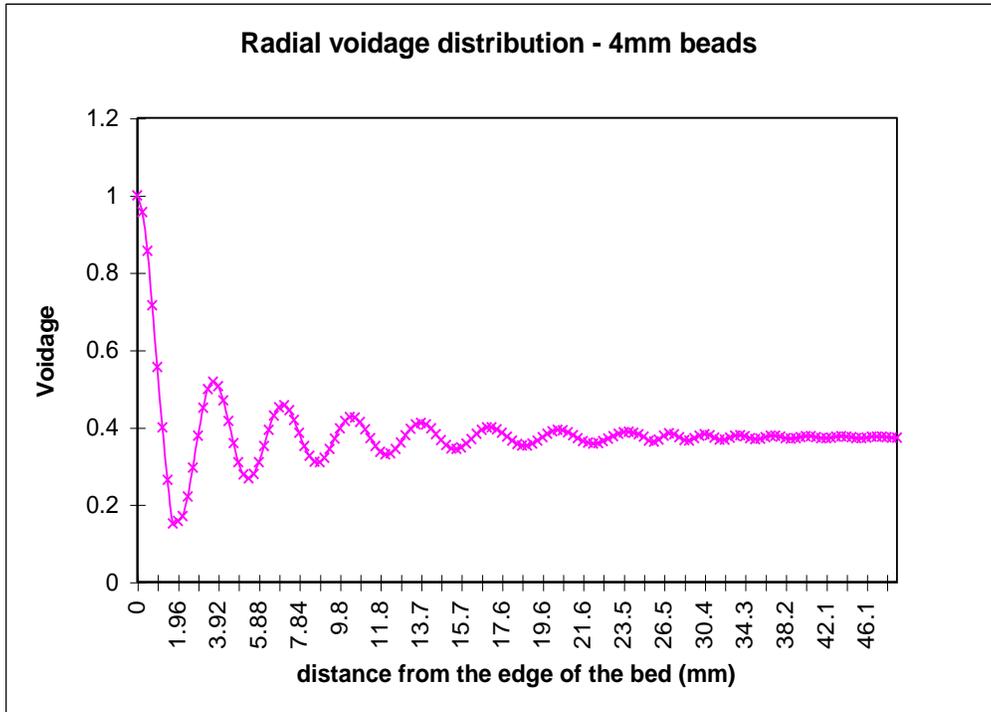


Figure 1: Typical radial voidage distribution

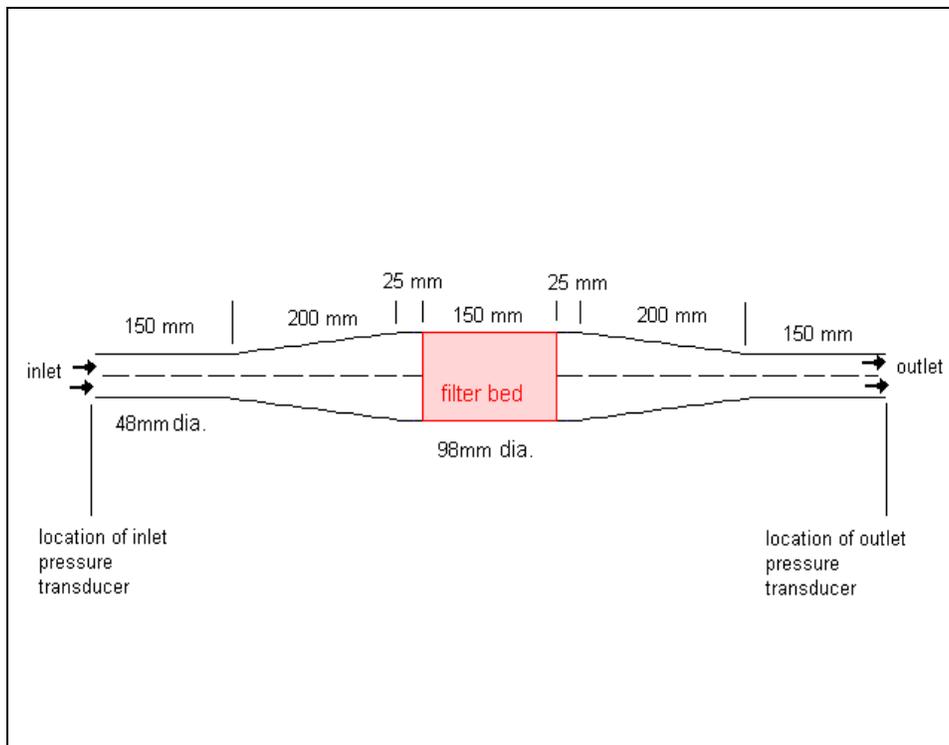


Figure 2: schematic diagram of filter geometry

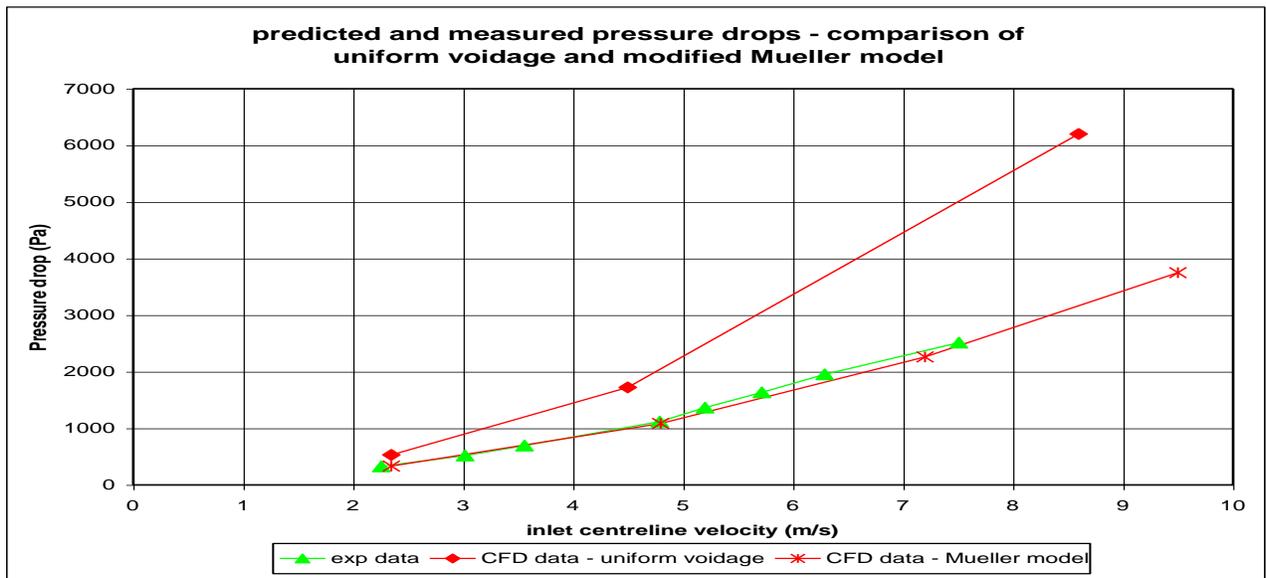


Figure 3: predicted and measured pressure drops for 3mm beads

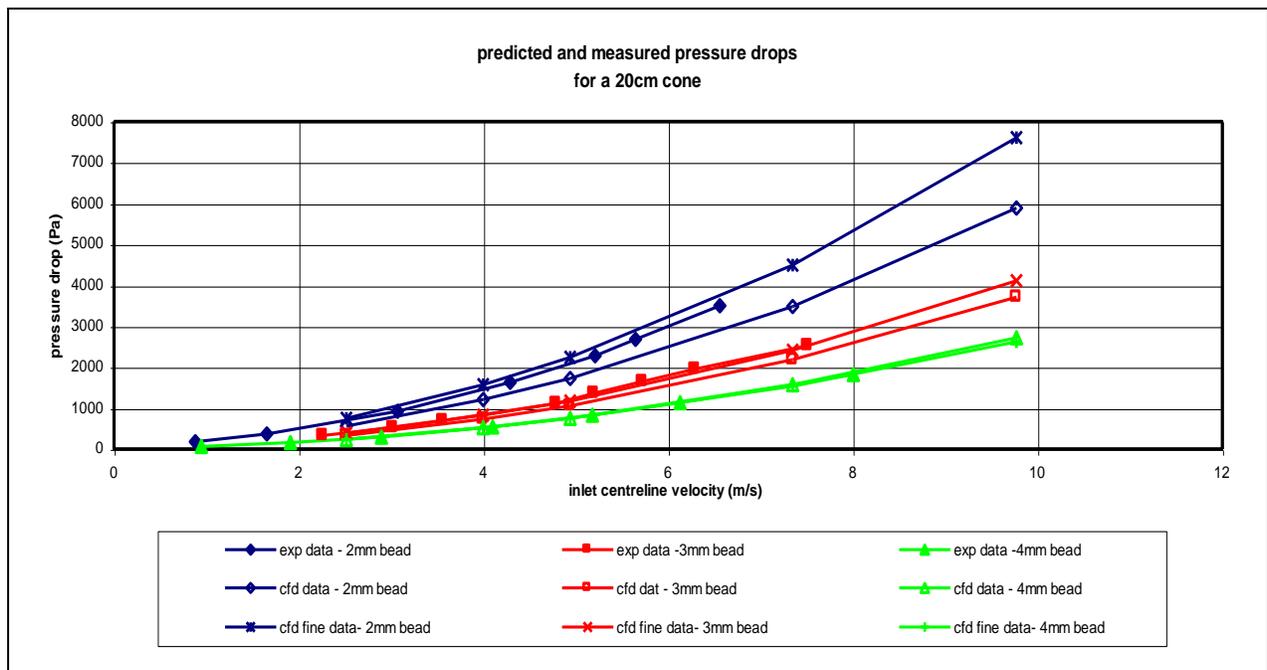


Figure 4: predicted pressure drop for 2, 3 and 4mm beads

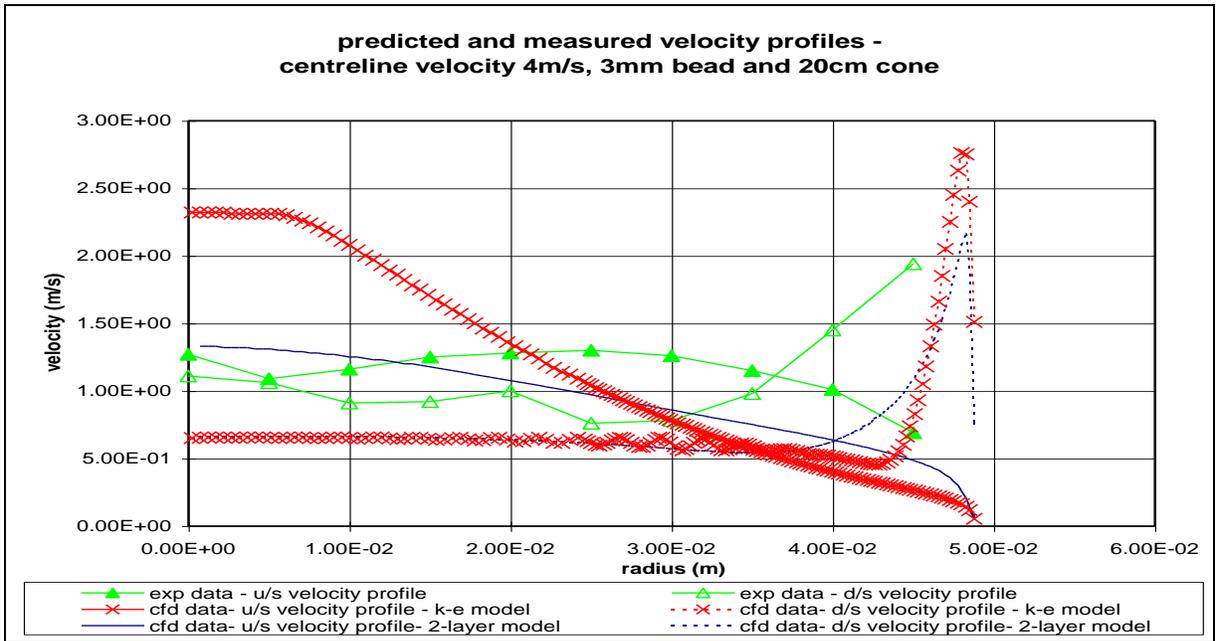


Figure 5: predicted velocity profiles with 20cm cone

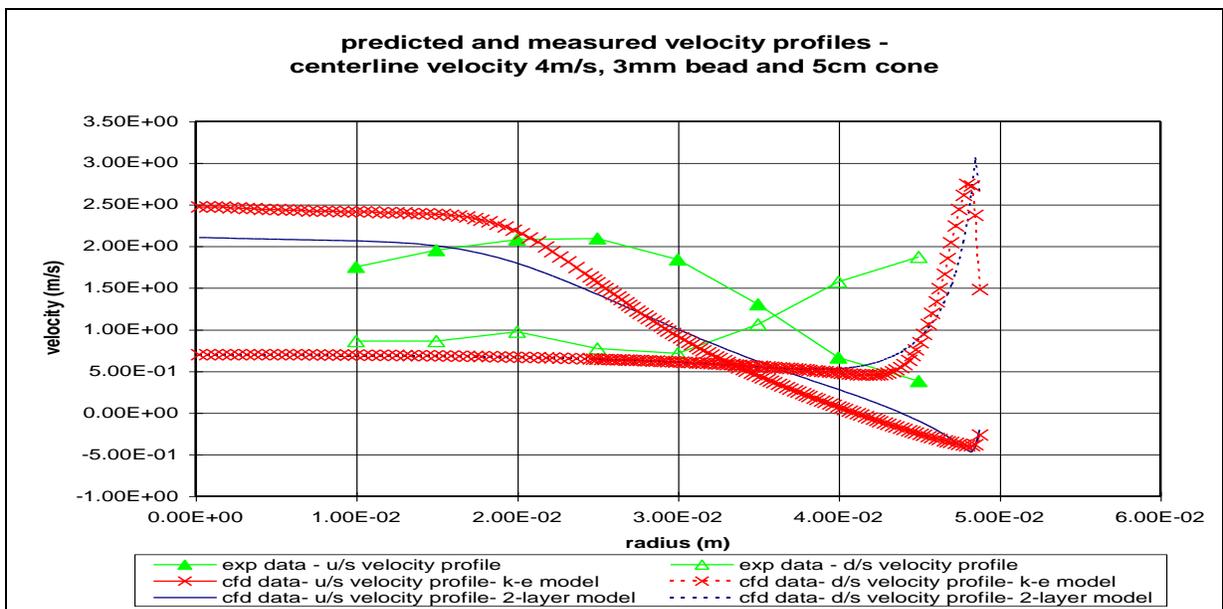


Figure 6: predicted velocity profiles with 5cm cone

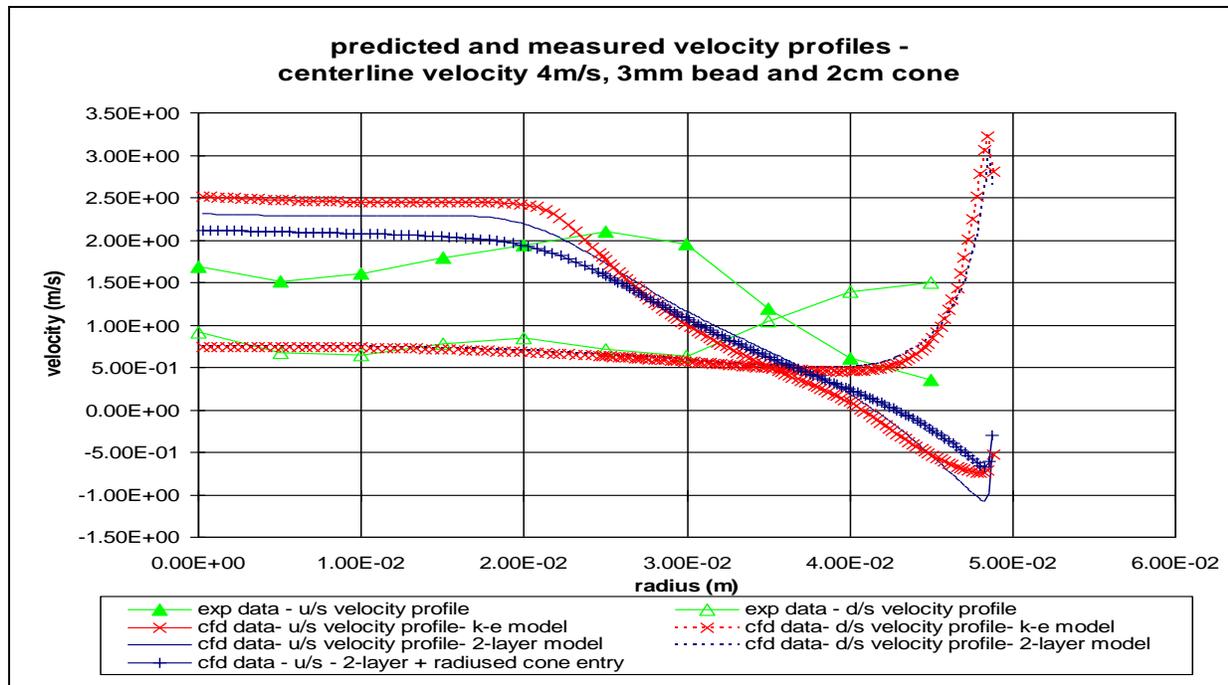


Figure 7: predicted velocity profiles with 2cm cone

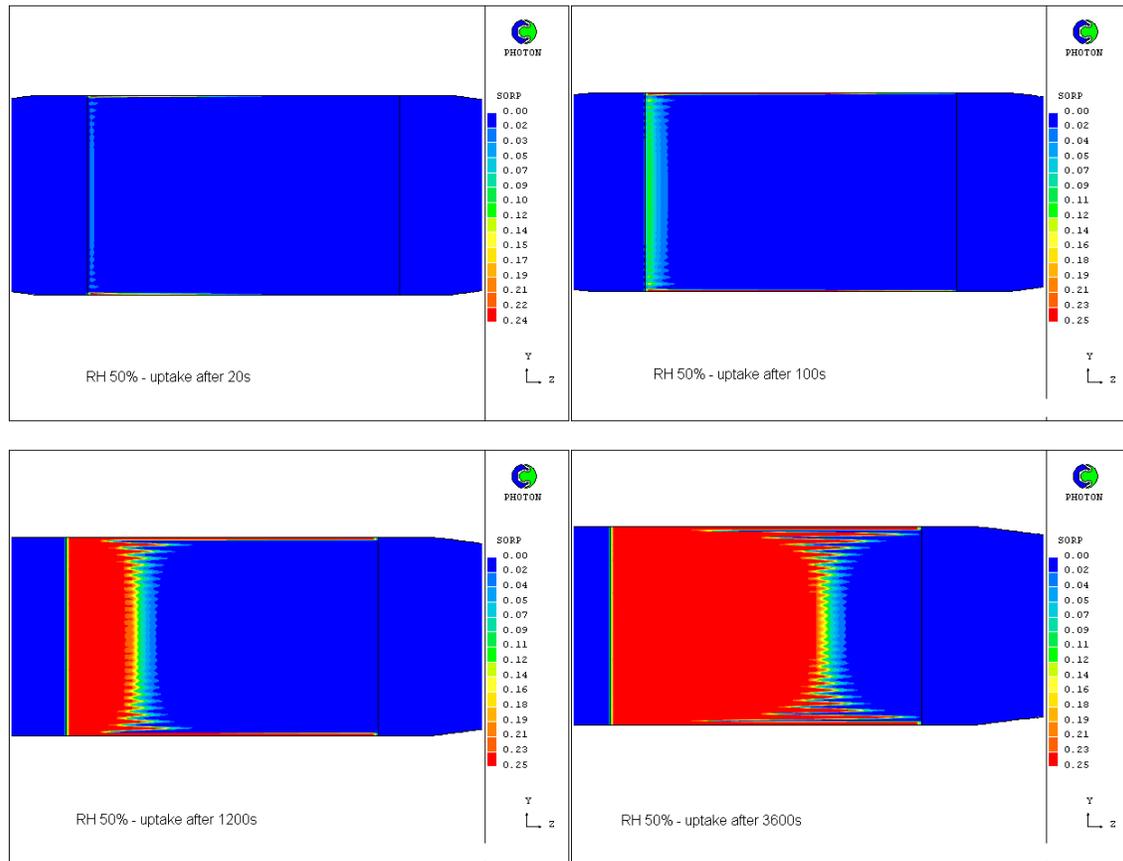


Figure 8: water uptake in filter bed at various times for 50%RH inflow