Software for Simulation and Modelling of Separation Processes

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abstract

Modern developments in computing have led to new techniques for the analysis of operating data, and for the simulation of industrial equipment. For example, a conventional approach to filtration analysis was to obtain certain filter cake properties and to predict throughput using analytical expressions relying on these average properties. Nowadays, the availability powerful personal computers has resulted in analytical expressions that can be evaluated at small increments during cake formation. Thus, in a full filtration analysis filter cake properties can be allowed to vary, as they do in practice. Hence, using a simple computer spreadsheet, it is possible to consider the deposition of filter cake in a layer-by-layer manner and to recalculate the filter cake properties at each stage. This approach is important when dealing with compressible filter cakes such as clays, finely divided particles and flocculated minerals. The techniques and equations for the simulations are described, and comparisons with laboratory results are illustrated, and demonstrate the advantages of this approach. The mathematical analysis employed is based on the so-called "modern" filtration theory, developed by Professors Tiller and Shirato during the 1960's. Both constant pressure and constant rate filtrations can be modelled in this way.

Simulation of the batch sedimentation of compressible compacts is also possible using an appropriately coded computer spreadsheet. The governing equation for this type of sedimentation is a non-linear parabolic partial differential equation that must be solved by a numerical technique such as Finite Difference. This has been achieved using a spreadsheet, and examples of how to use the simulation and the results are provided and compared with data taken during batch sedimentation of compressible compacts whilst monitoring the local concentration within the vessel using an electrical conductance technique.

The simulations can be used to investigate and illustrate practical operating conditions. For example, when filtering cakes that are compressible under constant pressure filtration conditions a move to short filter cycle times may improve productivity, but could result in filter cakes of poor discharge characteristics due to the nature of the resulting filter cake. The simulation may be used to investigate this type of performance.

The spreadsheets are freely available from an Internet web site and can be downloaded without registration or any other means of restriction of use and control.

INTRODUCTION

Simulation and modelling of solid/liquid separation equipment and techniques have been of interest to engineers and academics for many years. Initially, the calculations on which these processes depend had to be performed by hand. From the 1960's to the middle of the 1980's the wide scale application of computers and then microcomputers provided a welcome tool for such work, but required the use of high level programming languages in order to complete the work. In the late 1980's the computer software companies provided spreadsheet packages that could be readily used by novices, had the facility to recalculate values rapidly and provide a visual display of the results in a variety of graphical forms. The different spreadsheets had a very similar feel and method of use, as does any software operating under WindowsTM on a Personal Computer (PC). These developments have led to the wide scale use of spreadsheets in simulation and modelling of engineering application, including those relevant to filtration and separation^(1,2). The tools for analysis have improved beyond all measure in 30 years, however, someone is still required to set the model up inside the spreadsheet, check the results, etc.

The phenomenon of the 1990's has been the growth of the World Wide Web (WWW), or Internet. Its impact on humanity has been compared with that of printing in the 15th century. This may be an understandable exaggeration, but few would argue that it will not continue to grow at an astounding rate and have a major effect on business and lifestyles in the future. From its origins in an academic related free-for-all, the Internet has had a reputation for being a source of information, data and even programs that cost nothing to download and use. This is now changing as larger commercial organisations perceive a market opportunity, but there is still a vast amount of useful material freely available on the Internet, including some interesting work related to filtration and separation. This paper describes simulation and modelling of solid/liquid separation using computer spreadsheet files that are freely available to anyone who wishes to download them from a given WWW site⁽³⁾.

ANALYTICAL TECHNIQUES AND FILE DESCRIPTIONS

Eight spreadsheet files are currently available. Further details, including the compressed file size, are included in Table 1 and a more comprehensive description of the theoretical basis of some of the spreadsheets may be found elsewhere⁽⁴⁾. The first three spreadsheets in the table are straightforward and require little explanation.

Table 1 Files that may be downloaded from http://www-staff.lboro.ac.uk/~cgrgh/

File name	Zip file size (kB)	Brief description
specific	12	Specific surface area per unit volume, specific resistance to filtration and filter cake permeability calculated from a particle size distribution.
conpress	10	Calculates specific and medium resistances from experimental constant pressure filtration data.
exponent	11	Calculates the exponents and constants in the simple Lewis power law model relating concentration and resistance to cake forming pressure from experimental data.
rvf	12	Simulation under different operating conditions on rotary vacuum filter, assuming incompressible cake filtration.
conrate	21	Simulation of constant feed rate filtration of a compressible filter cake- which does not give a constant filtrate rate because of compression effects.
filter	75	Simulates constant pressure filtration of a compressible filter cake and illustrates the point that the pressure forming the cake in not constant as the cake builds up.
profile	26	This uses the same solution technique as the above file but provides information on the local solid concentration profile within the forming filter cake.
sediment	109	A Finite Difference simulation of batch settling of a compressible sediment, with graphical output to check convergence of solution.

incompressible cake filtration

The rotary vacuum filter (rvf) simulation of a has been described before⁽¹⁾, but this is an up-dated version that requires input in terms of specific resistance rather than the originally reported cake permeability. The basis of the solution starts with the well known parabolic rate law equation

$$\frac{t}{V} = \frac{\mu\alpha c}{2A^2\Delta P}V + \frac{\mu R_m}{A\Delta P} \tag{1}$$

where *t* is filtration time, *V* is filtrate volume, μ is liquid viscosity, α is specific resistance *c* is the dry cake mass per unit volume filtrate, *A* is filtration area R_m is filter medium resistance and ΔP is the pressure drop over both the filter cake and the filter medium. The dry cake mass per unit volume filtrate is usually calculated from the following equation

$$c = \frac{s\rho}{1 - sm} \tag{2}$$

where s is the mass fraction of solids in the slurry and m is the cake moisture ratio (mass of wet cake over mass of dried cake). In the simulation equation (1) is solved as a quadratic equation using filtrate volume as the independent variable, given inputs including filtration time and



physical properties. The filtration time comes from the fractional submergence of the drum and the rotation speed. Thus the simulation can be used to investigate the effect of changing typical operating parameters such as these, and others such as applied filtration pressure (vacuum) and effect due to slurry preconcentration before filtration. If the solid density is known cake depth may also be

Figure 1Effect of slurry preconcentration on RVF throughputdepthmayalsobeoperating conditions: drum speed 1/3 r.p.m., fractional submergence 0.3, total drumcalculated.Thislastarea 1 m^2 , total filtration pressure 64.4 kPa, liquid viscosity 1 mPa s, liquid density 1000 factor may be importantkg m^{-3} , specific cake resistance 2.2x10¹¹ m kg⁻¹, cloth resistance 5.53x10⁹ m⁻¹, solidin order to ensuredensity 2650 kg m^{-3} and moisture ratio 1.8.adequatecake

discharge. Other calculated values displayed in the spreadsheet include dry solids throughput, slurry mass throughput and slurry volume throughput as functions of operating variables. An illustration of the simulation is provided in Figure 1, where the effect of pre-concentration of the slurry before filtering was investigated. All the other operating conditions are provided in the text following the figure. The figure illustrates the considerable significance of feed slurry preconcentration on filtration performance. The downloadable spreadsheet file has been written in a way that makes alteration of the operating conditions easily achieved, hence this simulation may be used to investigate a variety of options supplied by the user.

compressible cake filtration

A simulation of constant rate filtration of an incompressible material is relatively straightforward. However, the constant rate filtration of a compressible material is not. The feed to the filter may well be essentially at constant rate, using a reliable positive displacement pump for example, but in order to achieve this the operating pressure will rise and have a consequent influence on the cake properties and filtrate rate. Compression effects will increase the filter cake solid concentration and specific resistance, and liquid from the old layers of compressing cake will report to the filtrate in addition to that coming from the newly forming layers. In order to model this situation the constitutive relations in the following two equations must be known.

$$\alpha_{av} = \alpha_o (1-n) \Delta P_c^{\ n} \tag{3}$$

$$C_{av} = C_o (1 - u) \Delta P_c^{\ a} \tag{4}$$

where α_{av} and C_{av} are the values for specific resistance and cake volume concentration averaged over the full filter cake, α_o , C_o , n and u are empirical constants and ΔP_c is the pressure drop forming the filter cake.

In the simulation increments in operating pressure are considered: at each increment the cake properties are considered constant, but allowed to vary between each increment. Any error associated with this approach can be minimised by reducing the step size (in pressure) between the increments. The solution uses arbitrary values of overall pressure drop, which increase during the constant rate filtration, and calculates the time interval corresponding to the increase in pressure. The starting point is Darcy's law which may be written as

$$\frac{\Delta P_n}{L_n} = \mu \alpha_{av} \rho_s C_{av} \frac{\delta V}{\delta t} \frac{1}{A}$$
(5)

where ρ_s is the solid density, ΔP_n and L_n are the pressure drop over the newly formed layer of filter cake during an increment and the depth of that layer. A material balance on the depositing solids gives

$$L_n A \rho_s C_{av} = Q C_s \delta t \rho_s \tag{6}$$

where Q is the feed rate of suspension and C_s is the feed concentration as a volume fraction. Equation (6) can be rearranged for L_n and substituted into equation (5) to give

$$\Delta P_n = \mu \alpha_{av} \rho_s Q C_s \delta V / A^2 \tag{7}$$

The incremental filtrate volume is equal to the product of the filtrate volume flow rate (q) and the incremental time difference

 $\delta V = q \delta t$

which can be substituted into equation (7), and gives the following equation after rearrangement for time

$$\delta t = \Delta P_n (A^2 / \mu \alpha_{av} \rho_s q Q C_s)$$

Note that q is the filtrate flow rate and Q is the feed flow rate, thus q < Q. The filtrate flow rate can be deduced from the feed flow using a knowledge of the filter cake and slurry volume fraction concentrations and a mass balance. It is equation (8) that is solved for time increments using the selected pressure increments. The full solution scheme is illustrated in the flow diagram given in Figure (2).

(8)

The flow chart illustrated in Figure 2 is relevant to a spreadsheet implementation of the simulation, where circular references to cells are permitted. Thus the incremental time is required for the calculation of the new total cake height which, in turn, is used to calculate the incremental time. The iteration is easily performed on a spreadsheet and requires no intervention by the user, whereas a computer program would require a loop in order to iterate a converged solution for the correct incremental time. The most significant assumptions in this method of solution are:

- 1. R_m remains constant throughout the filtration,
- 2. cake pressure drop comes from the total pressure drop minus that over the medium at the previous time increment (this limits the step size), and
- 3. the properties of the newly formed cake layer (concentration and specific resistance) are similar to the average filter cake properties.





Note that δt is required here but not calculated until later - a spreadsheet allowing circular references can be used for the calculation or iteration is required when using a computer program.

Figure 2 Flow sheet for calculations during compressible cake constant rate filtration

SIMULATION RESULTS

There are two illustrations for constant rate filtration, Figures 3 and 4. The former figure shows how the filtrate rate actually increases slightly due to cake compression during filtration. The second figure shows how the filtration pressure, required to maintain the constant feed rate filtration, changes during the process.



Figures 3 and 4 Simulations during an apparently constant rate compressible cake filtration

operating conditions: constant feed rate 70 litres per minute, total filter area 9.4 m^2 , slurry concentration 0.05 by mass fraction, liquid viscosity 1 mPa s, liquid density 1000 kg m^{-3} , n=0.5, u=0.08, $\alpha_o=4.5x10^8$, $C_o=0.15$, cloth resistance $1x10^{11} m^{-1}$, solid density 2800 kg m^{-3} .

During the constant rate filtration of incompressible material the filtration pressure rises linearly with time, or volume of filtrate produced. However, the non-linear response of constant (feed) rate compressible cake filtration can be seen illustrated in Figure 4. As the pressure increases the cake responds by becoming more resistant to fluid flow, through compression effects, hence the pressure required to maintain the feed rate increases non-linearly. The downloadable file includes a full printout of cake properties, and the filter cake concentration varies from 27% v/v to 38% v/v over a period of 43 minutes during the filtration. The average cake specific resistance to filtration varies by an order of magnitude over the same time interval.

One further notable point on Figure 4 is that the pressure with time curve does become almost linear after an extended filtration time, but an extrapolation of this line to the intercept of the dependent variable axis would result in a negative value. This illustrates a significant problem when a moderately compressible material is treated as being incompressible (i.e. assuming a straight line relation between pressure and time): the value of this intercept is conventionally used to calculate the filter medium resistance. Negative values of the intercept have no physical meaning and are of no use in the calculation of medium resistance. Hence even moderately compressible materials should be modelled in an incremental way, as described above.

The simulation of compressible cake filtration under conditions of constant pressure has been

described previously⁽²⁾, and an incremental approach to cake formation has been performed by many filtration researchers^(5,6,7). However, the illustration of the application of this simulation included here (and the file called *filter*) is used to illustrate the early stages of cake formation and its importance to filter operation. The operating conditions used in the illustration are applicable to a rotary vacuum filtration of a moderately compressible material, with a compressibility coefficient of 0.5. Figure 5 shows how the pressure drop over the cake increases from zero; i.e. all the pressure drop is over the filter medium to start with, rising to a value of just over 50 kPa after 2 minutes (the blue curve on the figure). Thus the total filtration pressure may remain constant at 65 kPa but the distribution of that pressure drop will vary significantly during the early stages of filtration. The filter cake is compressible, hence the average cake concentration will also vary over the same time period. However, as the exponent value in equation (4) is relatively low, only 0.08 in the example used, the cake concentration reaches an approximately constant value



Figure 5 Apparently constant pressure filtration

operating conditions: total filter area 1 m², total filtration pressure 65 only a limited cake depth is achieved kPa, liquid viscosity 1 mPa s, liquid density 1000 kg m⁻³, slurry under these conditions: see the results concentration 0.15 by mass fraction, n=0.5, u=0.08, $\alpha_o=4.5x10^8$, from the next simulation. It is worth $C_o=0.15$, cloth resistance $8x10^{10}$ m⁻¹, solid density 2650 kg m⁻³. reflecting that under these conditions only 30% of the applied vacuum for

the filtration is actually going to form the filter cake, the rest draws the filtrate through the cloth. Further insight into the performance of constant pressure filtration of compressible cakes can be gained by considering the calculated local concentration profile within the forming filter cake.

The *profile* simulation applies a similar solution mechanism to that used in the above: to calculate the instantaneous filtrate flow rate by iteration, allowing the cake properties of specific resistance and concentration to vary between iteration. A full description can be found elsewhere⁽²⁾. However, this simulation is designed to investigate the solid concentration profile within the forming filter cake, and displays the result as local concentration as a function of height from the filter medium, see Figure 6. The origins of the theory used in these compressible cake simulations are due primarily to the work of Tiller and Shirato and are well documented^(4,8,9). The data used to construct Figure 6 was identical to that used in Figure 5, so both illustrations are

well before that of the pressure drop over the cake: after approximately 10 seconds. All the values used in this illustration are realistic ones, coming from experimental measurements⁽⁴⁾.

A filtration time of 10 seconds on rotary vacuum filter a is equivalent to the time taken to form the cake during the drum's cycle. Thus the rotation speed of the drum employing this cake form time will depend on the submergence of the drum: if the drum operates 25% at submergence then it will take 40 seconds for a full cycle or be rotating at 1.5 rpm. However,



relevant to а simulation of the same filtration and use realistic values. The height of the filter cake after just 10 seconds of filtration can be seen to be only 2 mm, which is unlikely to give satisfactory cake discharge. Furthermore. the rheology of cakes, pastes and suspensions is such that it is usual for cakes to be very loose up to a threshold value of

Figure 6 Local concentrations from simulation

concentration. Above that threshold

the cake would be firmer and discharge more readily. In the absence of some testwork it would be impossible to say if this material is above or below that threshold after 10 seconds filtration, but if that value is known, or can be estimated, then the downloadable simulation could be used to investigate suitable operating conditions required to achieve that condition. Two further filtration times are considered in Figure 6: cake form times of 30 and 60 seconds, corresponding to drum speeds of 1/2 and 1/4 rpm respectively. When filtering a material such as that illustrated it can be seen that very slow drum speeds are required in order to obtain filter cake heights suitable for discharge by a scraper. The slow drum speed will also result in a more concentrated cake more likely to have the right rheological properties for discharge.

In order to use the simulations provided by the profile and filter files the operator will have to know the values for the constitutive relations: equations (3) and (4). Thus some experimental work is still necessary, but simple laboratory batch tests should be capable of providing the data to predict the performance of process scale equipment using the above simulations. In the absence of test data an estimate of equipment performance could be obtained using published values of these constants⁽⁴⁾, selecting the ones most similar to the application under investigation.

Sedimentation of compressible compacts

Simulating the batch sedimentation of a compressible sediment requires the application of a numerical solution to the differential equations representing the process. One of the earliest papers to describe the numerical analysis of sedimentation was published in the early 1970's⁽¹⁰⁾. At that time the settling vessel could only be divided into a few elements and a numerical approximation technique was used in a computer program for the solution. One of the advantages of modern computer spreadsheets is the ability to recalculate, or iterate, values on the spreadsheet until a convergent set of results are formed. This makes the application of spreadsheets appropriate to numerical solutions of differential equations by means of the mathematical technique of finite

difference. The file *sediment* uses a 'three time level method' of finite difference in order to solve the partial differential equations for batch sedimentation. This method of solution converges by considering values before and after as well as at the time increment under investigation. It may be thought of as a spreadsheet table in which the result in a cell are dependent on the values in all the immediately surrounding cells; in this instance the rows represent variation in time and the columns variation in amount of material (related to the concentration) in an element. One advantage of a spreadsheet is that it is easy to copy and paste cells, thus the number of elements that the vessel may be split into for the solution can be adjusted easily, to either improve the accuracy of the result or to speed up the solution, as necessary.

The spreadsheet requires eight pages in the spreadsheet notebook file for solution, and a further page is used to assist in the representation of the height of the settling interface and concentrations within the sedimentation vessel. Each one of the pages has mathematical functions that must be evaluated, and used on other pages, in order to arrive at the converged solution. The mathematical description of these functions, including the equations and their method of solution can be found elsewhere⁽¹¹⁾. This paper is concerned with the use of the spreadsheet for the purposes of simulation and to provide information to engineers who may wish to download the file and apply it to their investigations.



Figure 7 Batch sedimentation of compressible compacts: spreadsheet page

The first page of the file contains all the inputs necessary in order to complete the simulation, an example of it is shown in Figure 7. All the inputs prior to running the model are contained in the region above the asterisks on the spreadsheet; i.e. row 10. Physical properties of the solid and liquid are required: densities, liquid viscosity and specific surface area per unit volume of the particles in suspension. The latter may be obtained from the first spreadsheet described above. Information on the suspension also needs to be entered: the initial slurry concentration in volume fraction terms and the initial suspension height. The coefficient and exponent required in cells D6 and D7 are the same values as those used in equation (4) above, and may be obtained using the spreadsheet *exponent*. The other parameter dependent on the solids under investigation is the initial Kozeny constant. This is the value of the Kozeny constant at the slurry concentration prior to sedimentation. During sedimentation the Kozeny constant has, in fact, been found to be a variable dependent on concentration⁽¹²⁾, often approaching the expected value of 5 at high concentrations when settlement has ceased. As a first approximation towards the modelling of a batch sedimentation a value of 5 may be used, if there is no experimental data for this parameter. The remaining values above row 10 are in cells C8 and C9; these represent the

step size used in the finite difference solution and they can be left unaltered in all cases.

In the region below row 10 all the calculated values are given. Initially the data is turned into a non-dimensional form using factors calculated in rows 12 to 15. Thus all the values supplied in the table, row 18 and beyond, are non-dimensional and need to be converted back to values with readily understandable physical meaning. Thus column C, from cell C21, contains non-dimensional time, which needs to be converted back to real time in column A. Inserted on top of the table of results is a graph to illustrate how the suspension/supernatant interface settles with time. Prior to starting the numerical solution off, using the spreadsheet, this graph should display a horizontal line at a value equal to the given initial suspension height. During the process of iteration to find the solution this interface curve can be seen to move slowly downwards, until it alters no more; indicating that the iterative solution has converged. In order to use the spreadsheet two further cells are important, H16 and K16. When an alteration is made to the spreadsheet, such as putting in new values above row 10, change cell H16 to 0. This should reset the spreadsheet to its initial condition, i.e. before sedimentation occurs, and the cell K16 should read the same value as the initial concentration entered in cell D3. Depending on the alteration

made it is sometime necessary to iterate once or twice in order to complete the reset procedure: this can be accomplished by pressing the key labelled F9. The numerical solution within the spreadsheet is activated by changing the cell value in H16 to 1, and then iterating until convergence. Convergence can be checked by viewing the inserted graph, or by looking for only a small alteration in the value given in cell K16. This cell shows the concentration close to the top of the settled sediment, which is the last position within the batch sedimentation column to come



<u>Figure 8</u> <u>Simulation of batch sedimentation – results compared with measurements</u> to an equilibrium value. The example illustrated in Figure 7 shows a solution after convergence. The iteration procedure can be achieved by several methods including: repeatedly pressing the iterate key [F9] or by presetting the number of iterations before activating the initiator cell (cell H16).

The spreadsheet has been used in a number of batch sedimentation simulations, one such is illustrated in Figure 8, which compares the modelled and measured results for the batch sedimentation of a suspension of the mineral talc. The suspension/supernatant interface curve was measured visibly, whereas the solid concentrations below the interface were measured using electrodes positioned within the vessel to measure electrical resistance, which were calibrated to solid concentration. Both the predicted interface settling curve and the solid characteristics rising up from the base of the sedimentation vessel closely matched the experimental measurements.

DISCUSSION

All the simulations were developed using the Quattro Pro v5 spreadsheet package. However, most have been up-dated into Microsoft Excel Office'97 format. The simulations can be downloaded in zip format in order to speed up transfer. The equations and approaches used in the simulations have been validated over many years, but they have limitations. These are due to the application of the theory beyond its limit rather than problems with the computer files. For example, the approach of compressible cake modelling using equations (3) and (4) in order to provide the cake concentration profile works well with materials of up to moderate compressibility; n values of less than about 0.7. At higher values the approach is no longer valid, hence the computer simulation will provide incorrect results just as a hand calculation would. In practice, cakes made from ground materials, precipitates and fine particles such as clays can be simulated this way but cakes made from very fine solids and biological sludges are unlikely to be modelled successfully. When acceptable filtration theories for such materials become available spreadsheets to analyse and simulate them will be possible.

In many cases the correct assessment of the filter medium resistance is essential. In the case of apparently constant pressure filtration it is the filter medium resistance that causes the cake forming pressure to become a variable with respect to time. If the medium resistance is negligible then all the pressure drop will be across the forming cake and, for a constant pressure filtration, the filter cake properties should not, therefore, change with time. Thus an incremental analysis would not be required. Filters that are cyclic and with short run times are unlikely to operate with completely negligible filter medium resistance. Hence, this parameter is a very important operating variable and one that is critical to a successful filtration simulation. This subject has recently received significant quantitative analysis^(13,14), and an incremental approach to filter cake simulation could be modified to include the effect of changing filter medium resistance during the initial phase of the filtration cycle.

CONCLUSIONS

Simulation of filtration and sedimentation can be readily achieved by the application of well known quantitative relations described in many text books. It may be implemented by computer program or by setting up a model in a computer package such as a spreadsheet. The latter has the advantage that iteration is readily performed and the result of the simulation can be easily displayed in a graphical, and visual, format. Some simulation files for compressible cake filtration and batch sedimentation are available at no cost by downloading them from an Internet Web site. Simulation enables the operator to assess the effect of a variable change before attempting that change with the operating equipment: it is ideal for performing a "what-if" type of process analysis. Simulation can also help to explain the observed effects on existing equipment. For example, in some instances there is a trend towards thin cakes and rapid cycle times; simulation shows that this will increase productivity. However, a more detailed simulation showing filter cake concentration profiles may show that the cake depth becomes too small, and the cake

concentration too low, to enable adequate cake discharge. Thus simulation can be used to explain the occurrence of "sloppy" cakes that are difficult to discharge. Hence, simulation assists in the understanding of a process and focuses attention on the important physical parameters influencing filtration and sedimentation.

Accurate simulation does rely on reliable constituent relations, models and variable values appropriate to the process under investigation. The latter should be obtained from some existing data, operating or laboratory, the relations and models are constantly under investigation and revision from the academic community. The provision of high speed and low cost computing power has led to the adoption of simulation in an incremental, or layer by layer, approach to the problem.

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