COMPUTER SOFTWARE FOR THE SIMULATION OF SOLID/LIQUID SEPARATION EQUIPMENT

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ABSTRACT

This paper details aspects of Filter Design Software® (FDS), Windows® software for the selection and simulation of solid/liquid separation equipment as well as the analysis of test data. FDS has been developed in collaboration with multi-national companies spanning a wide range of industrial sectors to provide a comprehensive calculation, education and training tool that maintains a balance between ease of use, level of knowledge conveyed and comprehensibility.

The selection module of the FDS compares up to 7 user-defined selection criteria with information contained in databases to produce a numerically ranked list of potentially suitable equipment. The FDS allows access to text and pictorial descriptions of more than 70 equipment types and hyperlinks provide more specific equipment manufacturer details via the internet.

The data analysis module facilitates interactive analysis of leaf filtration, jar sedimentation and piston press test data. Calculations are performed in a hierarchical manner using the available information, if some data are not measured then the FDS performs the best possible analysis using approximations. The results of an analysis can be used to refine (shorten) a list of selected equipment or provide scale-up information for equipment simulation.

Results in the paper concentrate on the equipment simulation capabilities of FDS. More than twenty types of vacuum and pressure filters can be simulated which potentially involve combinations of cake formation, compression and gas deliquoring, and washing. By way of example, the operation of a pressure Nutsche filter that is required to process a pharmaceutical product is simulated and the predicted influence of crystal formation and other operating parameters on the filter cycle are shown. Simulations quantify how crystal form can detrimentally influence all phases of a cycle and lead to, for instance, slower filtration and wetter cakes.

KEYWORDS

Equipment selection; Software; Solid/liquid separation; Simulation; Analysis of filtration data; Process design.

INTRODUCTION

The specification of filters is generally performed through rules-of-thumb (or heuristics) rather than by applying fundamental theoretical relationships. Equipment is rarely specified without recourse to extensive laboratory and pilot scale tests, and the data produced can lead to erroneous specification and scale-up of separators unless care and consistency are observed. The lack of a standard approach can lead to the poor specification and sizing of filters with the result that required production rates may not always be achieved and unforeseen difficulties arise in filter cycle operations.

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Progressive developments have facilitated a combined theoretical and experimental approach to the use of computer software in filter specification and simulation[1-3]. The philosophy considers that with the present state of knowledge of suspensions, and their behaviour in separators, it is most appropriate to have interactive computer software that forms an integral part of an experimental program (Figure 1). Within this context the Filter Design Software[4] (FDS), designed to run under Windows®, was developed.

The FDS is a sequence of interlinked modules that can be used independently from one another. The full set of FDS modules offers many capabilities, including:

- A catalogue and explanation of the main operational and design features of 70+ equipment types and a procedure for ranked equipment selection
- Full analysis capabilities for leaf filter, jar sedimentation and expression test results to give the parameters required for scale-up and simulation of solid/liquid separation equipment
- Comparison of data sets from a range of tests or trials
- Simulation of 20+ types of vacuum and pressure filters
- The ability to import data files from other software (e.g. spreadsheets)
- Web access to equipment suppliers.

SIIMULATION MODULES

This paper concentrates on the simulation capabilities of the FDS and two modules are currently available. The Vacuum Filter module allows for the simulation of Nutsche, multi-element leaf, belt, drum, disc, table and tilting pan filters. The Pressure Filter module is able to simulate single and multi element leaf filters, diaphragm and filter presses as well as the tube press. Figure 2 shows an example screen display for the simulation of a pressure Nutsche filter.

Key Features

The 'General Information' box toward the top left hand corner of the display is used to start a simulation procedure. The cycle configuration is defined here. For a vacuum filter this may comprise combinations of cake formation, washing and gas deliquoring whilst variable volume filters may also incorporate a cake compression phase. The FDS prevents impractical stages on particular filters, for instance, cake washing on a rotary disc filter. The Unit file allows the user to specify their preferred units for data entry and the default washing model can be over-ridden by the specification of an experimentally measured wash curve.

The remainder of the information required for simulation is typed by the user in the 'Simulation Data' box toward the top right hand corner of the display. Each 'tab' corresponds to a phase in the filter cycle or provides facility to enter data specific to the filter or the feed solids, liquid and solute. The results of a simulation are shown towards the bottom of the display.

Features of the Vacuum and Pressure filter simulation modules include:

- Simulation of the different modes of cake formation as determined by the type/method of pumping used (constant pressure, constant flow and variable pressure/variable flow), compression and cake post-treatment processes (cake washing and cake deliquoring)
- Checking of input data – for each required entry the FDS displays a range of numerical values to guide the user as to what is realistic for a particular filter

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- Where possible the simulation calculation sequences within the FDS are hierarchical - depending on which data are missing, a sequence of assumptions are made in order to carry out the calculation
- The FDS takes account of practical constraints, for example, the minimum cake thickness that can be discharged from a particular filter
- Graphical or tabulated output of results
- On screen display of a process mass balance, indicating the input/output amounts of solid, liquid, and dissolved solute components
- The ability to save results to disk for later recall and viewing in spreadsheets.

EXAMPLE OF FDS COMPUTER SIMULATION

Problem

A pressure driven Nutsche filter is to be used to separate batches of a crystalline pharmaceutical product (see Figure 3) from a propanol based suspension. Variations in upstream formulation mean that crystallisation of the *β*-form, which is more difficult to filter, can occur in place of the *α*-form. In each batch, 50 kg of solids are present at a concentration of 6% v/v and it is envisaged that cake formation will occur to a maximum depth of 50 mm. In order to meet product specifications this new filter installation requires a sequential cycle comprising filtration, displacement washing and gas deliquoring. Preliminary tests in the laboratory suggest that the cake formed in each cycle needs to be treated with 3.5 wash ratios of pure propanol to remove unwanted solute residues after which deliquoring (with pressurised nitrogen) proceeds for 1500 s to dry the cake ready for discharge with the plough.

The characteristics for both the *α* and *β* particle forms in suspension have been determined experimentally and these are shown in Table 1 along with other suggested operational parameters.

For the *α*-form, determine the required filter area, the solid, liquid and solute throughput rates, the filter cycle time and other performance indicators. Assess the impact on the filter cycle if *β*-form crystallisation occurs.

Solution

Repeated use of the FDS facilitates a solution to the example problem; more details are provided elsewhere[1,2].

With the *α*-form of crystal, the required filter area is 2 m^2 for the specified 50 kg of solids per batch and 50 mm cake thickness. Each cake discharged from the Nutsche contains ~16.6 kg of propanol and (theoretically) no undesirable solutes. A total of 637 kg of propanol passes through the filter per batch, including 178 kg of wash liquid and 5.14 kg of solutes are removed with the filtrate (4.57 kg) and washings (0.57 kg). As shown in the bottom row of Table 2, the total cycle time is 2775 s.

With reference to Figure 3 and Table 1, the *β*-form of crystal is more acicular (needle-like) and forms a cake of higher compressibility as evidenced by the constitutive equations for cake resistance and solids volume fraction. If a sequence of calculations are performed for the *β*-form with the 2 m^2 Nutsche then the results shown in Table 2 are obtained. Due to different intrinsic properties, a cake containing 50 kg of solids exhibits a thickness of 47.4 mm rather than the 50 mm observed with the *α*-form. The approximate four fold increase in specific cake resistance with the *β*-form more than doubles the total cycle time and leads to a significantly wetter cake at the end of deliquoring (i.e.

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28.6% compared with 24.9% for the α-form). To achieve a 24.9% moisture content would require either a deliquoring time of ~4300 s at the original 200 kPa pressure or a raised deliquoring pressure of 480 kPa applied for the specified 1500 s. The implications of processing the β-form of particle are significant in terms of either longer cycle times and/or raised equipment specification.

It is evident that a reduced maximum cake thickness would lead to reduced filtration and deliquoring times, albeit at the expense of a larger filter area and the potential limitation of increased channelling (during washing) with excessively thin cakes. Conversely a thicker cake would lead to a smaller filter but longer processing times.

CONCLUSIONS

This paper has described the principal features of the Filter Design Software with a particular emphasis on filter simulation. The modules comprising the software, which can also be used in isolation, have been developed to enable:

1. A selection procedure that facilitates ranked listing and access to on-line equipment and process information from a knowledge of the required duty and basic experimental data

2. The consistent analysis of filtration, expression and jar sedimentation tests to allow the accurate determination of the parameters required for process simulation and the basic information needed for equipment selection

3. The detailed simulation of process scale batch and continuous filters involving combinations of filtration, consolidation, washing and deliquoring.

By doing so a number of benefits arise, including:

1. The ability to investigate new plant and ask 'what-if' questions about filter installations to facilitate optimum equipment selection(s), filter sizing, cycle configuration(s) and filter operation

2. The ability to troubleshoot existing filter installations and identify potential solutions

3. Consistent experimental data analysis to give characterisation and scale-up parameters

4. Unbiased information on solid/liquid separation equipment so appropriate manufacturers can be approached in the early stages of equipment selection

5. The ability to educate and train a user in solid/liquid separation technology.

ACKNOWLEDGEMENTS

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REFERENCES

1. Wakeman R.J. and Tarleton E.S., 2005, *Solid/Liquid Separation: Principles of Industrial Filtration*, xii + 330 pages, Elsevier, Oxford.

2. Tarleton E.S. and Wakeman R.J., 2006, *Solid/Liquid Separation: Equipment Selection and Process Design*, 464 pages, Elsevier, Oxford.

3. Wakeman R.J. and Tarleton E.S., 2005, *Solid/Liquid Separation: Scale-up of Industrial Equipment*, xi + 454 pages, Elsevier, Oxford.

4. *Filter Design Software – Solid/Liquid Separation Equipment Selection, Design, Simulation, Education and Training*, 2005, Filtration Solutions, www.filtrationsolutions.co.uk

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TABLES AND FIGURES

Parameter	Value
Septum characteristics	
Filter medium resistance	4×10^{10} m^{-1}
Operating conditions	
Filtration, washing and deliquoring pressures	200 kPa
Solute concentration in the feed	9 kg m^{-3}
Particle and fluid properties	
Density of filtrate and wash	802 kg m^{-3}
Viscosity of filtrate and wash	0.0023 Pa s
Surface tension of filtrate and wash	0.025 N m^{-1}
Solute diffusivity	6×10^{-10} m^2 s^{-1}
Particle and cake properties specific to α-form	
Density of solids	1370 kg m^{-3}
Constitutive equations for filtration, Δp_f in kPa	$\alpha_{av} = 5.6 \times 10^9\ \Delta p_f^{\ 0.2}$ m kg^{-1} $C_{av} = 0.28\ \Delta p_f^{\ 0.05}$ v/v
Particle and cake properties specific to β-form	
Density of solids	1420 kg m^{-3}
Constitutive equations for filtration, Δp_f in kPa	$\alpha_{av} = 4.5 \times 10^9\ \Delta p_f^{\ 0.5}$ m kg^{-1} $C_{av} = 0.27\ \Delta p_f^{\ 0.06}$ v/v

Table 1: Characteristic parameters for the Nutsche filter simulation. Δp_f ≡ filtration pressure; α_{av} ≡ specific cake resistance; C_{av} ≡ cake solids concentration.

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Parameter	α-form	β-form
Filtration phase		
Duration (s)	707	2363
Specific cake resistance (m kg^{-1})	1.62x10^{10}	6.36x10^{10}
Cake solids volume fraction (v/v)	0.365	0.371
Cake thickness (mm)	50	47.4
Cake moisture content (%)	50.5	48.9
Washing phase		
Duration (s)	568	1959
Fractional solute recovery	1	1
Deliquoring phase		
Duration (s)	1500	1500
Final cake saturation	0.33	0.42
Final cake moisture content	24.9	28.6
Total cycle duration (s)	2775	5822
Total volume of liquids produced (m^3)	0.773	0.736

Table 2: Comparison of filter cycle performance for two particle forms in a Nutsche filter.
Δp_f = 200 kPa; A_f = 2 m^2.

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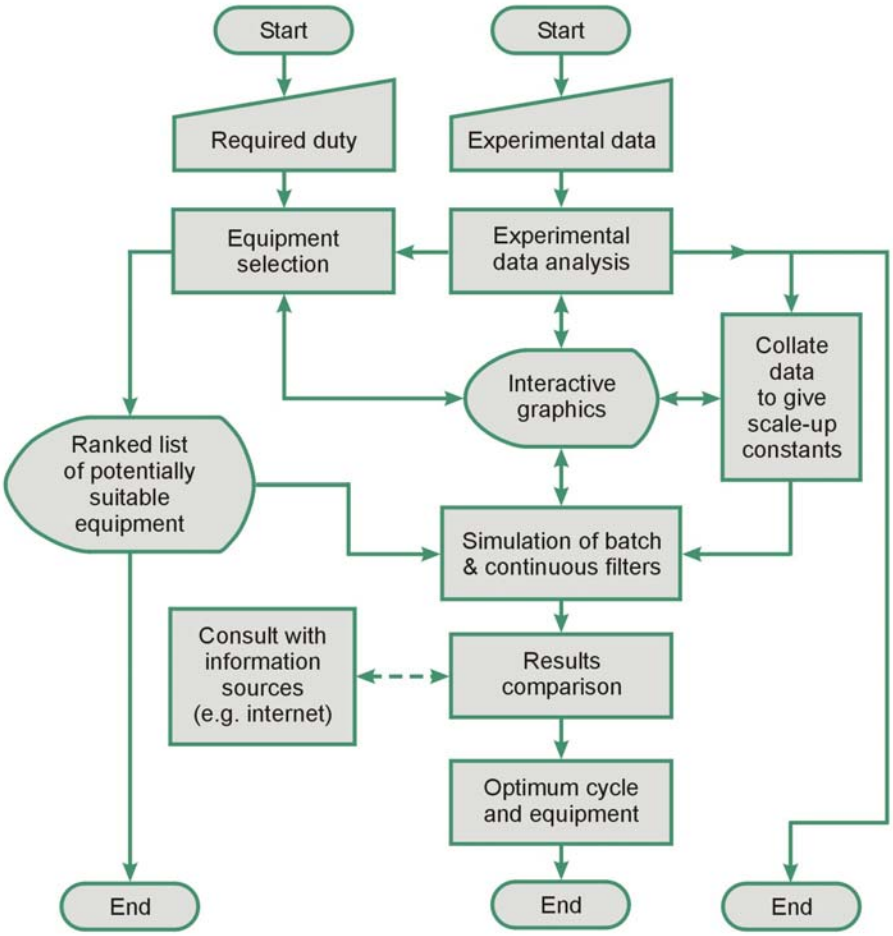

Figure 1: Flowsheet showing the integration of selection, analysis, scale-up and simulation in the Filter Design Software.

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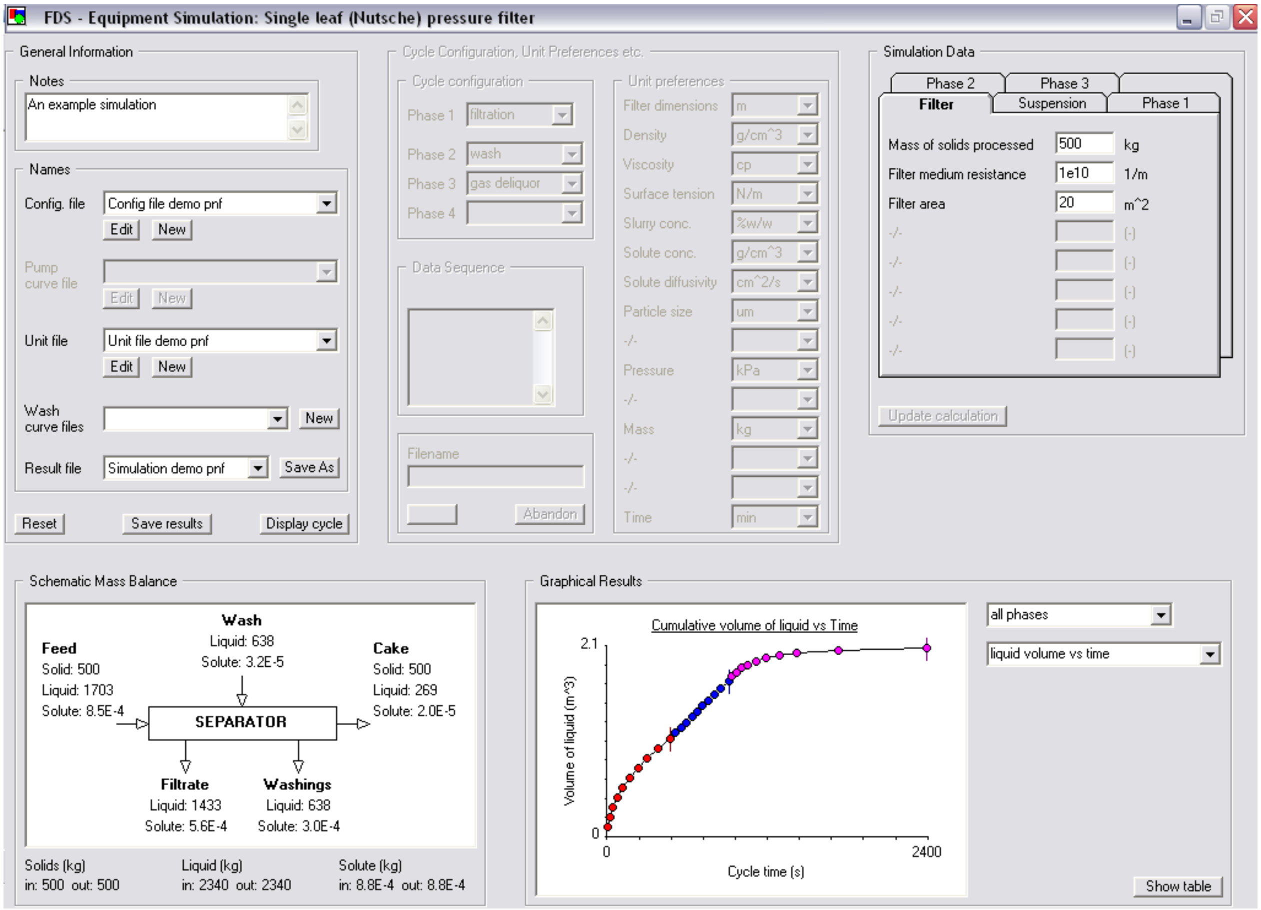

Figure 2: FDS screen display for a pressure Nutsche filter simulation.

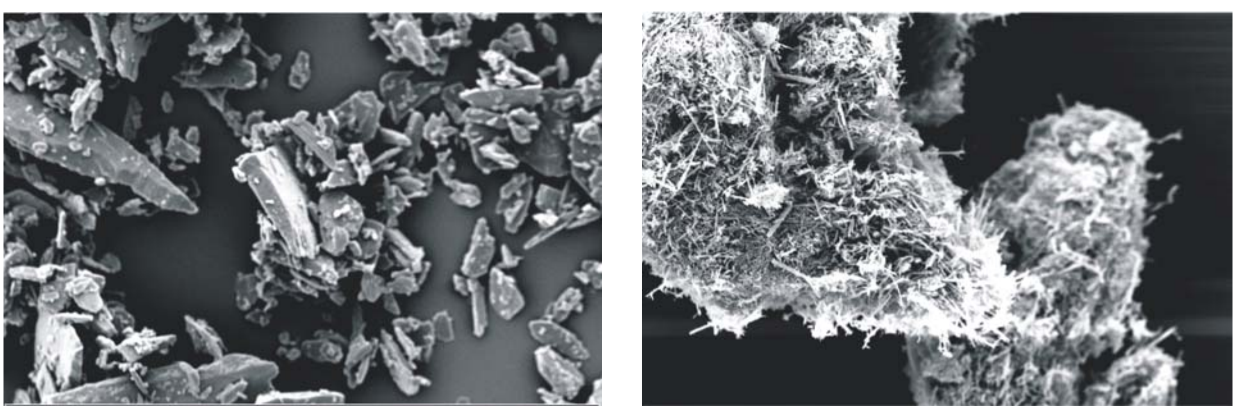

Figure 3: Scanning electron micrographs of two forms of crystalline pharmaceutical product; cubic, α-form, (*left*) and needle, β-form, (*right*).

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