Calculations of Flow in Evaporator with Solids Present at the Base – 11539

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ABSTRACT

Knowledge of the likely temperature distributions in Highly Active Liquor Evaporation and Storage (HALES) facilities is key to getting an assessment of the operational lifetime of these components. In particular, there is the potential for a layer of heat generating solids to accumulate over their operational life and therefore it is necessary to obtain accurate predictions of the temperatures within these layers to improve the lifetime corrosion assessment of the base components. The distribution of heat generating solid material and its behaviour when recirculating liquor flow impinges on any settled material is important in determining the heat distribution on the base of these vessels.

The physics of flow and heat transfer in the vessel is very complicated with only limited CFD analysis being done to date. The purpose of this work is to investigate the feasibility of using a rheology model within a single phase framework to model how solid material settled at the base is eroded in response to flows in an evaporator, assuming that the solid behaves like a viscous fluid.

Single phase modelling with the use of the Herschel-Bulkley model to represent the settled solid layer at the base has been used to model the erosion of the solid base layer in response to flows in an evaporator under typical operational conditions. Results of a parametric assessment of the Herschel-Bulkley model are presented. Illustrations are also given of replicating the viscosity profile of a homogenised Highly Active Liquor (HAL) simulant suspensions solution, and how stratification /layering in the solid material can be represented using the Herschel-Bulkley model in the current single phase approach.

Initial modelled results are encouraging, which indicate that the solid base layer can evolve in a physically intuitive manner with modest computing requirement.

INTRODUCTION

The temperature distribution on the base of an evaporator has important consequences with respect to the degree of corrosion expected over its operational life. The physics of flow and heat transfer in the vessel is very complicated with only limited CFD analysis being done to date. In particular, it is likely that the base of these tanks will have a layer of heat generating solids lying on them. It is therefore necessary to obtain accurate predictions of the temperatures within these layers to improve the lifetime assessment of the base components. The distribution of heat generating solid material and its behaviour when impinged by liquor flow is important in determining the heat loading and temperature on the base of these tanks. The purpose of the work described here is to determine how solid material settled at the base are eroded in response to flows in an evaporator, assuming that the solid behaves like a viscous fluid.

The object of this study is to determine conditions that could lead to an increase in the base temperature of evaporators and hence increase the corrosion rate. The plant is instrumented to enable good control of liquor and base temperatures; however this work will eventually enable a better definition of limiting conditions and help future plans to maximise throughput without detrimentally effecting corrosion.

This work builds on an initial modelling approach developed at the National Nuclear Laboratory to gain insight into the flow behaviour on the base of an evaporator using a simplified representation of the flow and the effects of boiling. Due to the approximate nature of the model, it is expected that only the broad trends can be represented although insight into the behaviours of the mobilisation of solids will be gained.

The work presented here demonstrates the feasibility of the proposed single phase modelling approach, with the use of the Herschel-Bulkley model, to represent the settled solid layer at the base to simulate the erosion of the solid base layer in response to flows in an evaporator under typical operational conditions. A parametric assessment of the Herschel-Bulkley model was carried out to examine sensitivity of the results to the viscosity model. . The model is further examined to assess its ability to replicate an experimental viscosity profile, and its potential to represent stratification/layering structures in some of the observed solid layers.

MODELLING ASSUMPTIONS AND APPROACH

This preliminary investigation uses a simplified representation of the flow and the effects of boiling on the flow, to establish the modelling approach/framework and get a functional model working. Details of the model components can be refined further if needed as more supporting experimental data becomes available in the future.

The modelled flow is assumed to be single phase and isothermal. The evaporator components are represented approximately (with porosity to represent blockage effects). As the blockages are not included explicitly in the model their effect is represented by appropriate porosity through the application of a flow resistance within a porous media model. This is implemented in FLUENT [1] by specifying the inertial loss coefficients. With the single phase assumption, the effect of boiling (on flow) is represented by momentum sources, whereas the solid layer settled at the base is modelled using a rheology approach by treating this region as a non-Newtonian power law (Herschel-Bulkley) fluid. The assumptions made in the modelling approach can be summarised below:

- The calculations are isothermal.
- The layer of solids (at the base) is represented using a rheology approach by treating this region as a power law (Herschel Bulkley) fluid.
- The fluid is entirely single phase with the effect of boiling represented by the application of sources of vertical momentum in the fluid.
- The liquor free surface is represented using a frictionless wall boundary condition.
- Coils (heating elements) are not included in the geometry explicitly but represented as porous zones with the appropriate blockage effect and flow resistances.
- Pipe work at the centre of the vessel (coil feed pipes and other tubes) is represented by a blockage effect.

The present study examines the flow in the evaporator using an axisymmetric model, but only considers the lower part of the evaporator that is occupied by the process fluid (i.e. excludes the ullage space) to investigate the erosion of the solid base layer in response to flows in an evaporator under typical operational conditions. With the axisymmetric assumption, only half of the evaporator geometry needs to be represented in the model. The overall geometry and main components of the evaporator considered are shown in Figure 1.

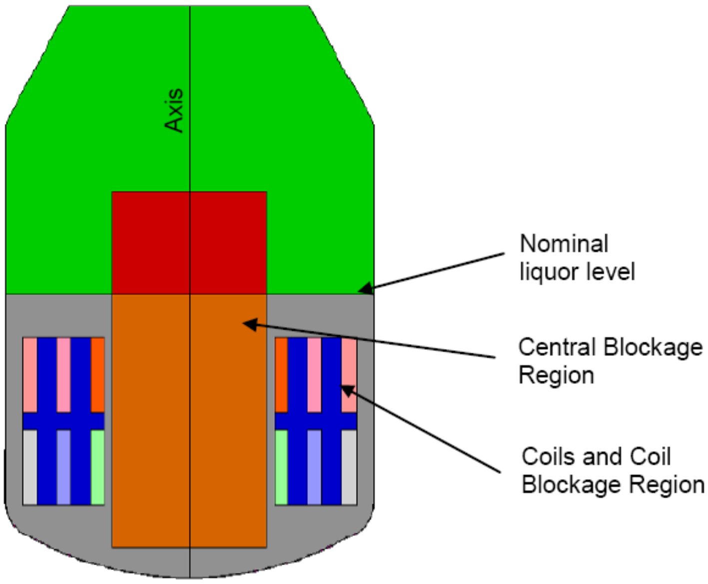


Figure 1 Overall geometry and main components of the evaporator.

HERSCHEL-BULKLEY MODEL

The representation of the solid base layer, as non-Newtonian fluid, using the Herschel-Bulkley Model in the present FLUENT model can be summarised as below. Bingham plastics are characterized by a non-zero shear stress when the strain rate is zero:

$$\bar{\bar{\tau}} = \bar{\bar{\tau}}_0 + \eta \bar{\bar{D}} \qquad \text{(Eq. 1)}$$

where τ_0 is the yield stress:

- For $\tau < \tau_0$, the material remains rigid.
- For $\tau > \tau_0$, the material flows as a power-law fluid.

The Herschel-Bulkley model combines the effects of Bingham and power-law behaviour in a fluid. For low strain rates ($\dot{\gamma} < \tau_0 / \mu_0$), the "rigid" material acts like a very viscous fluid with viscosity μ_0. As the strain rate increases and the yield stress threshold, τ_0, is passed, the fluid behaviour is described by a power law. Using the Herschel-Bulkley model for Bingham plastics the fluid viscosity can be calculated as:

$$\eta = \frac{\tau_0 + k[(\dot{\gamma})^n - (\tau_0 / \mu_0)^n]}{\dot{\gamma}} \qquad \text{(Eq. 2)}$$

where k is the consistency factor, and n is the power-law index (a measure of deviation from Newtonian flow with an index value 1).

Parametric study of the Herschel-Bulkley model

A systematic variation in the parameter values of the Herschel-Bulkley model (Eqn. 2) was carried out to assess the effects on rheological properties. Within the current Herschel-Bulkley model implementation, four parameters (i.e. τ_0, μ_0, k and n) are assessed by varying the values up and down by an order of magnitude. Table I summarises the settings used in the parametric study.

The computed viscosity and shear stress values are presented in Figure 2. It can be seen that the yield stress is the most influential parameter, with a near proportional relationship to the computed viscosity and a near proportional change in the computed shear stress for a decreasing yield stress, but a less than linear change from an increasing yield stress. The yield viscosity only has a small effect on the viscosity value (i.e. a 10 times increase in yield viscosity has little effect on viscosity, but up to ~20% reduction in viscosity for a 10 times reduction in yield viscosity), and a negligible effect on the shear stress. The effect of the consistency factor, *k*, on viscosity is small. Although at closer examination a highly non-linear behaviour is evident, such that a 10 times reduction in *k* causes a slight increase in viscosity at low shear strains (i.e. <50 s^{-1}), but leads to a decrease in viscosity at higher shear strain rates. The effect of *k* on the shear stress is small at low shear strain rates (e.g. <50 s^{-1}), but becomes more significant for high shear rates (e.g. >200 s^{-1}) especially for the case of 10 times increase in *k*. The effects of reducing the power-law index *n* from 1 to 0.6[1] is small on viscosity and shear stress, with the influence on the shear stress becoming more significant for high shear strain rates (e.g. >500 s^{-1}).

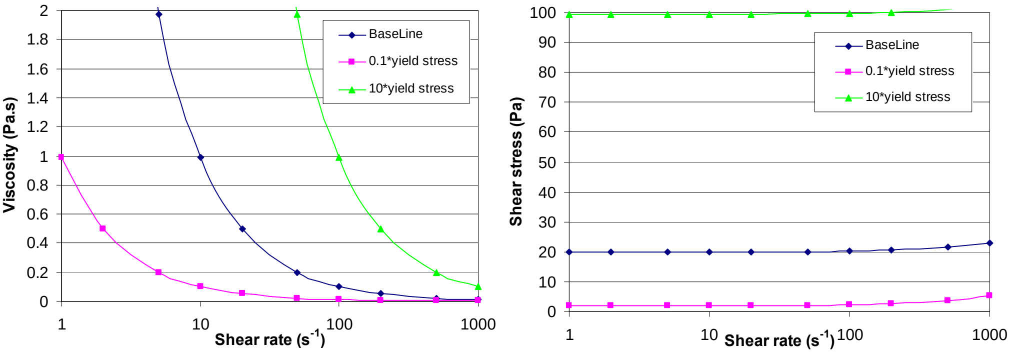
Table I. Parameter values of the Herschel-Bulkley models in parametric study.

RUNID (#)	BaseLine	RUN1	RUN2	RUN3	RUN4	RUN5	RUN6	RUN7	RUN8
Parameter variation (from Baseline)	-	0.1*yield stress	10*yield stress	0.1*yield viscosity	10*yield viscosity	0.1**k*	10**k*	0.8**n*	0.6**n*
τ_0 (Pa)	10	**1**	**100**	10	10	10	10	10	10
μ_0 (Pa.s)	0.2	0.2	0.2	**0.02**	**2**	0.2	0.2	0.2	0.2
k	3.25E-03	3.25E-03	3.25E-03	3.25E-03	3.25E-03	**3.25E-04**	**3.25E-02**	3.25E-03	3.25E-03
n	1	1	1	1	1	1	1	**0.8**	**0.6**

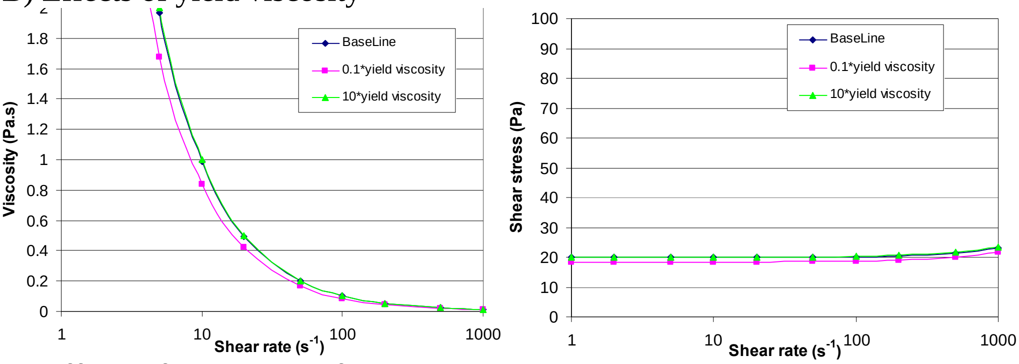
(#) Run identification used in the model runs presented in the result section below.

[1] *n* < 1 corresponds to shear-thinning behaviour typical of the sludge type flow consisting of sand/soil and water, which is believed to be of similar type to the solid layer considered here.

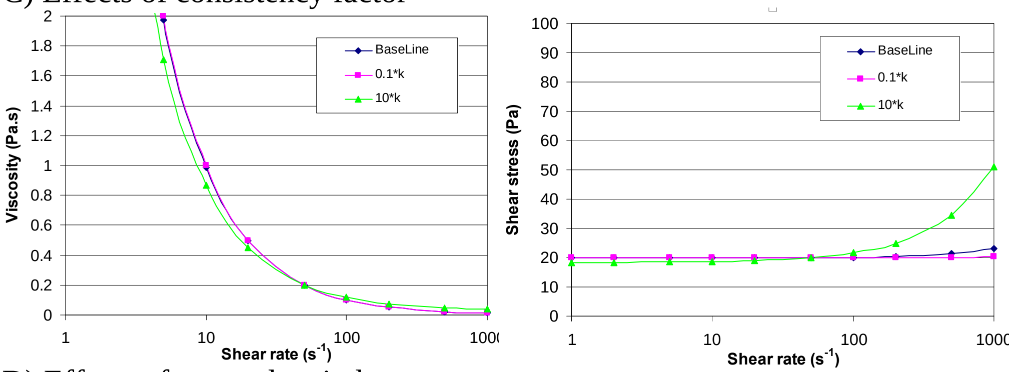
A) Effects of yield stress



B) Effects of yield viscosity



C) Effects of consistency factor



D) Effects of power-law index

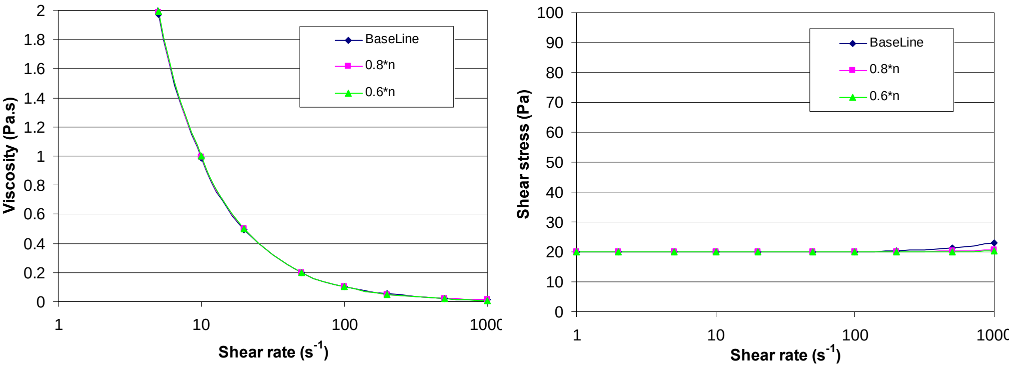


Figure 2 Effects of varying A) yield stress; B) yield viscosity; C) consistency factor and D) power-law index an order of magnitude up and down on viscosity (left) and shear stress (left).

Model results from Herschel-Bulkley model parametric runs

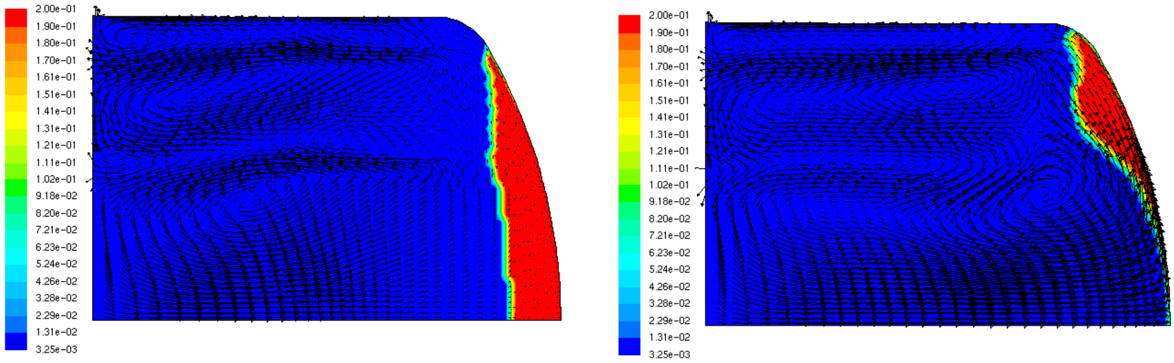
A systematic variation in the parameter values of the Herschel-Bulkley model was implemented in a series of model runs (see Table I). The Baseline case modelled result is used to provide a reference for the parametric runs to compare against (Figure 3).

With the axisymmetric flow assumption, the results are presented on a radial plane with the vertical axis of symmetry shown horizontally in the figures. The yield stress has a clear influence on the erosion of the solid base layer (see RUN1 and RUN2). Reducing the yield stress threshold effectively allows the erosion process to start working on the solid layer earlier (at a lower stress level) and results a more dispersed (broader) transition zone at the liquor-solid interface. The effect becomes more apparent over time (compare results of Baseline and RUN1 at 1 second).

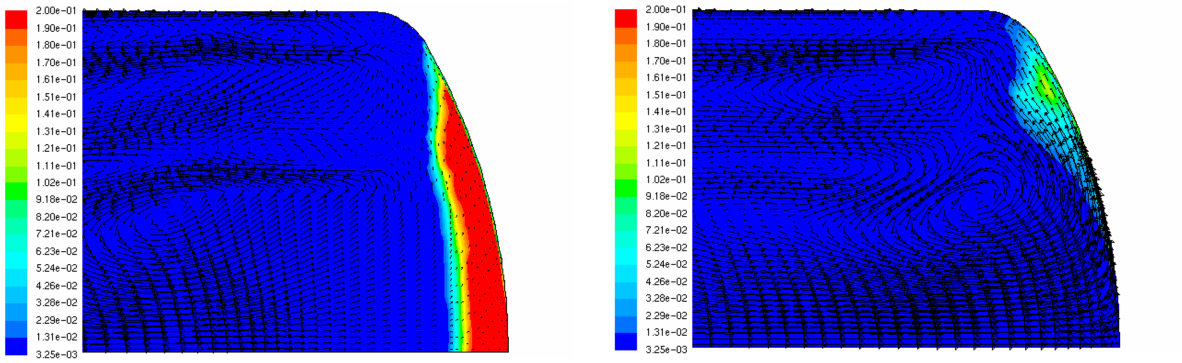
The yield viscosity has a noticeable effect on the erosion of the solid base layer (RUN3 and RUN4). Increasing the yield viscosity is seen to have a similar but smaller effect as decreasing the yield stress, causing a more dispersed zone at the liquor/solid interface. This can be realised from Equation (2) on the evaluation of viscosity, such that the yield viscosity appears as the denominator while yield stress is the numerator within a term with exponent n. The yield stress also appears as a single term which explains its more direct influence on viscosity.

The consistency factor seems to have a negligible effect on viscosity, giving visually near identical results (RUN5 and RUN6). For the range of power-law index examined here (i.e. 0.6 to 1.0), the effect on viscosity is negligible (compare RUN7 to Baseline). Result of RUN 8 was visually identical to RUN7 and is not shown here.

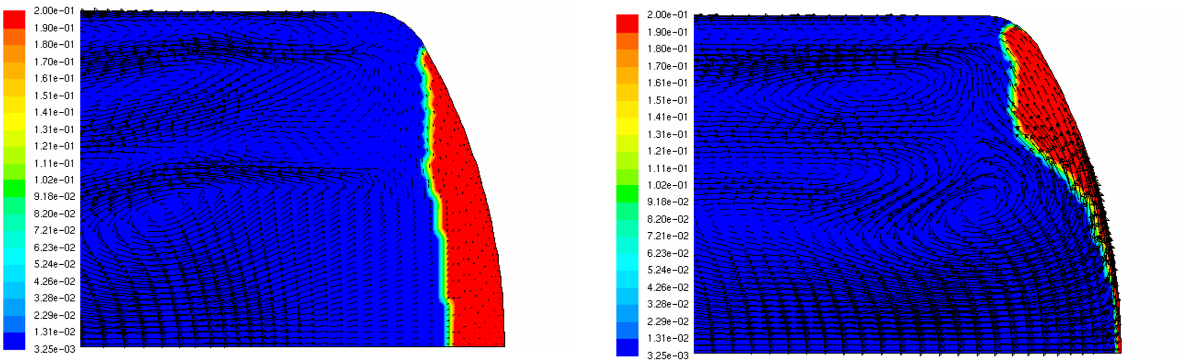
Baseline case



RUN1



RUN2



RUN3

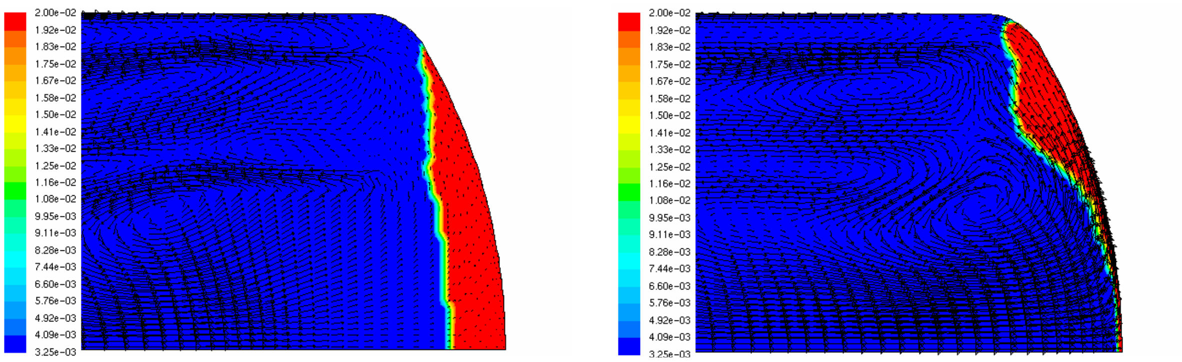
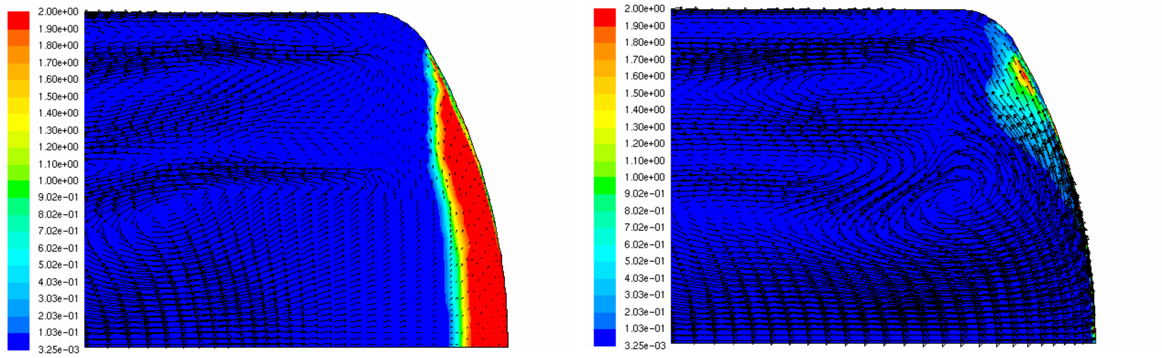
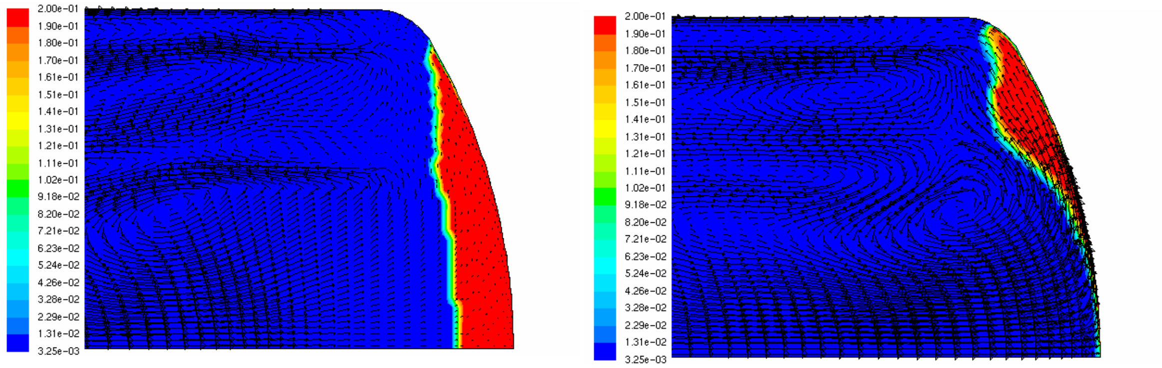


Figure 3 Contours of molecular viscosity (kg/ms) and velocity vectors at 0.5 second (left) and 1.0 second (right).

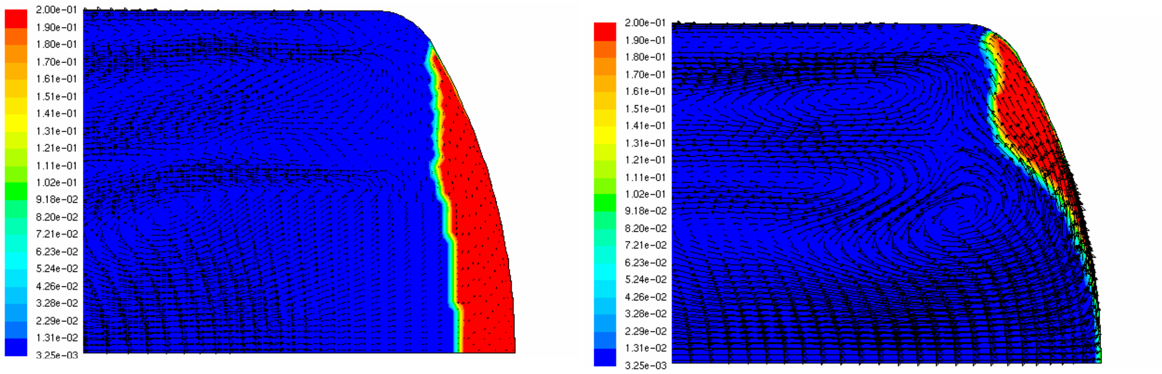
RUN4



RUN5



RUN6



RUN7

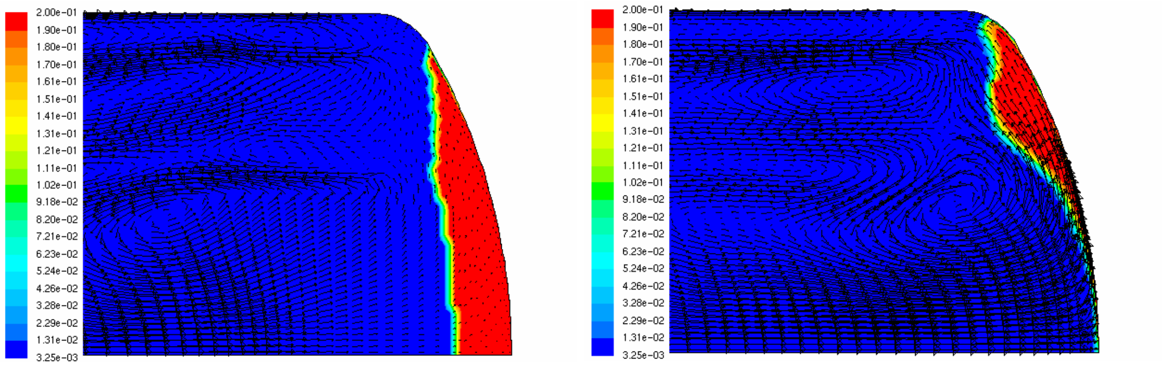


Figure 3 (Cont'd) Contours of molecular viscosity (kg/ms) and velocity vectors at 0.5 second (left) and 1.0 second (right).

Modelling with a closer alignment of rheological properties to actual solid solution

Attempts were made to adjust the parameters of the Herschel-Bulkley model to enable a closer alignment to actual measured data, to demonstrate the applicability of the model in a real life situation. For the purpose of illustration, a solid/liquor mixture of volume fraction of up to about 50% was used in the present study.

Attempts were made here to replicate the viscosity profile of a homogenised Highly Active Liquor (HAL) simulant suspensions at lower solid concentration of ~2 %wt/wt [2]. The spread of experimental shear viscosity profiles of a number of samples (indicated by block arrows) are shown in Figure 4 below for comparison with three Herschel-Bulkley models (namely Model-1, Model-2 and Model-3) using different parameter values as shown in Table II. The computed viscosity profiles indicate that both Model-1 and Model-2 agree well with the experiment. It's worth noting the same yield stress (the dominant factor identified in the parametric assessment) of 0.1 Pa is used in both models, while the other three parameters are different (allowing fine tuning of the model details). It should also be noted that the Baseline model shows a higher viscosity value, which is likely to be consistent with the solid layer that is expected to have higher (viscosity) values than the ones for the homogenised samples used here.

This highlights the need for data such as viscosity profile data for the solid layer, and therefore provides a focus for future experiments. Also more accurate determination of the yield stress is required as the factor seems to have significant effect on both the viscosity and shear stress values.

Table II. Parameter values for Herschel-Bulkley model.

	Baseline	**Model-1**	**Model-2**	**Model-3**
τ_0 (Pa)	10	0.1	0.1	1
μ_0	0.2	0.55	0.1	0.2
k	3.25E-03	1.63E-02	6.50E-03	9.75E-03
n	1	0.8	0.9	0.9

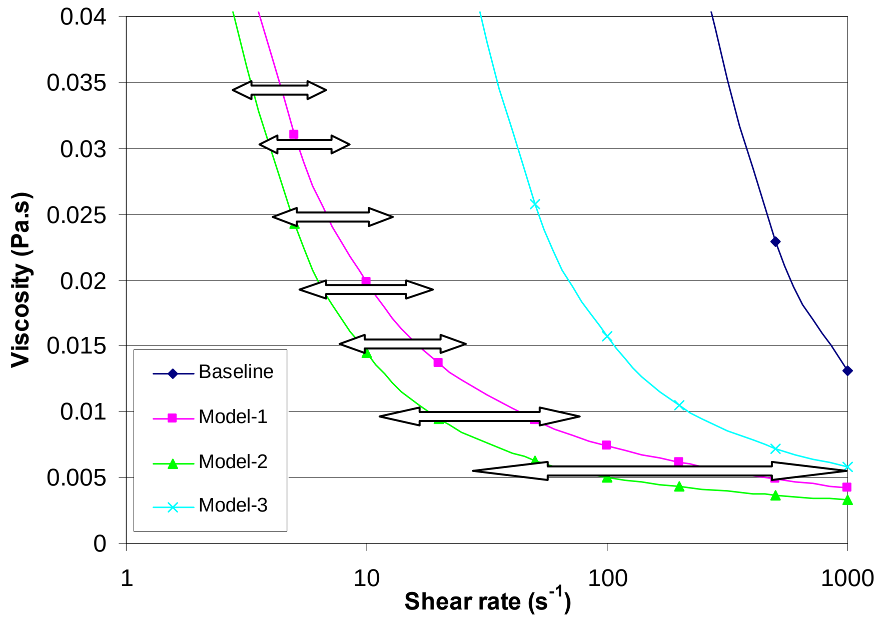


Figure 4 Viscosity profiles computed from Herschel-Bulkley model using different parameter values, with block arrows showing the approximate spread of measured profiles from a number of samples [2].

Model runs with representation of stratification in solid layer

In practice the solid base layer often consists of a number of solid phases, some being granular in nature that are likely to have variable particulate sizes, there are also evidence to suggest that stratified layering (or stratification) could occur [2]. An attempt was made to include representation of stratification in the base solid layer within the confines of the Herschel-Bulkley rheology model. Preliminary simulation of a base solid layer consisting of three layers/strata was performed to demonstrate the feasibility of such approach. The generic model contains three strata with increasing yield stress threshold towards the bottom. In this application the rheological parameters are assumed constant within a stratum (Table III). This is not a limitation of the model itself, which could easily be changed by using a user-defined variation should such a need arise (e.g. indicated by experimental data). The viscosity profiles of the strata represented in the 'stratification' model (Strata_RUN) are shown in Figure 5, also showing the Baseline case profile, indicating the broad range of viscosity characteristics represented in the solid layer.

Table III. The Herschel-Bulkley model parameters of the strata used in the model with stratification representation, also showing parameter values used in the Baseline case.

Stratum (#)	τ_0 (Pa)	μ_0 (Pa.s)	k	n	Stratum fractional thickness ($)
Statum_3	0.1	0.1	6.50E-03	0.9	0.3
Statum_2	1	0.5	9.75E-03	0.8	0.4
Statum_1	50	0.2	3.25E-03	0.6	0.3
Baseline	10	0.2	3.25E-03	1	1

(#) Stratum_3 is the top layer, Stratum_2 the middle layer and Stratum_1 the bottom layer.
($) The sum of fractional thickness of all strata should equal to 1.

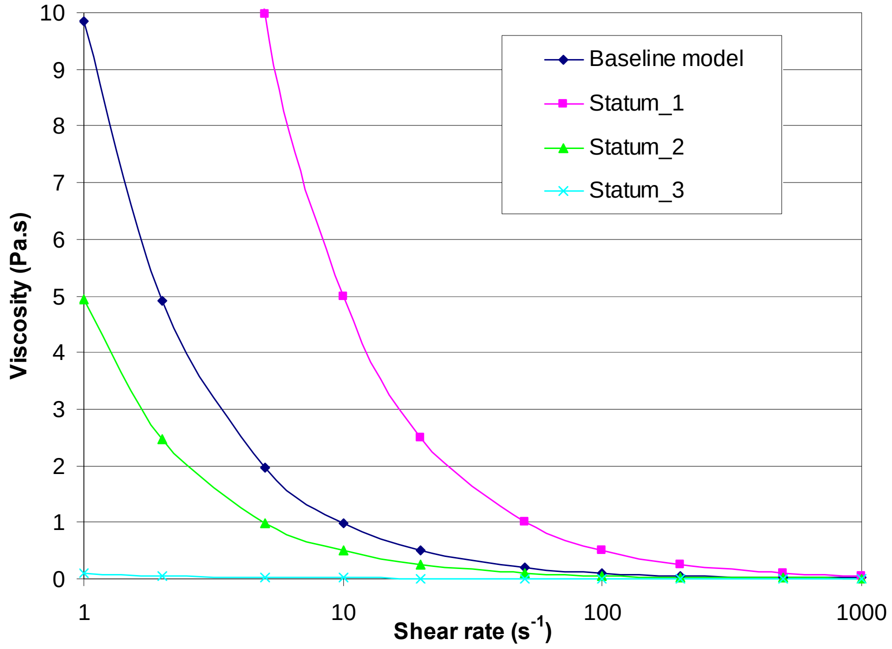
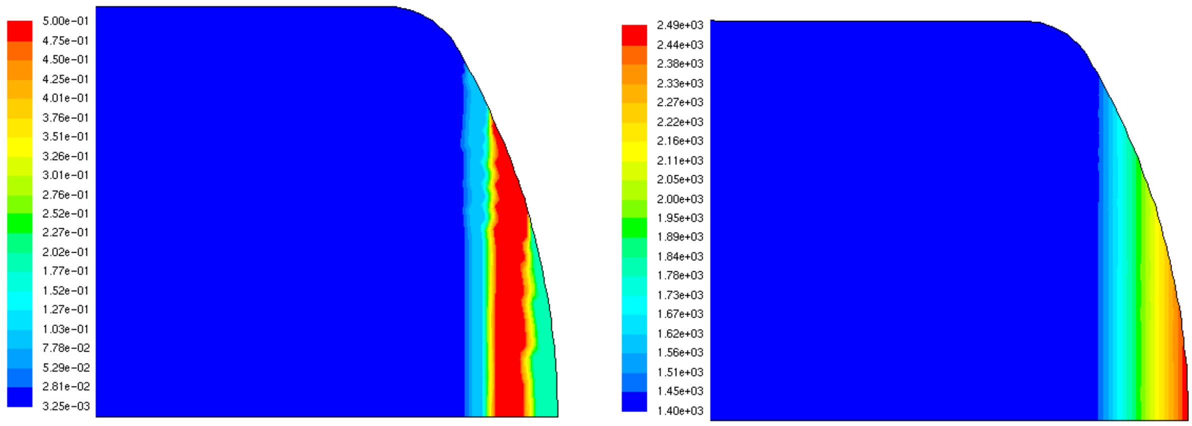


Figure 5 Viscosity profiles of the strata represented within the solid base layer, also showing the Baseline model profile.

The result of a transient simulation for the 'stratification' model (Strata_RUN) is shown in Figure 6. At time=0 second, the three strata are clearly seen from the viscosity contour plot. This simulation also uses the assumption of linearly increasing density over the solid layer depth. The evolution of the modelled viscosity, indicates a rather rapid erosion of the solid base layer due to the low yielding stresses of top strata. After 1 second signs of the high viscosity of the middle layer are still noticeable in the contour plot. This is expected to decrease and 'fade away' over time as erosion continues to work through the solid 'layers'. An appreciation of the transport of the bulk solid material at 1.0 second can be gained from the modelled density contours, showing the solid base layer being transported radially outward and swept towards the outer wall.

Time=0 second



Time=1 second

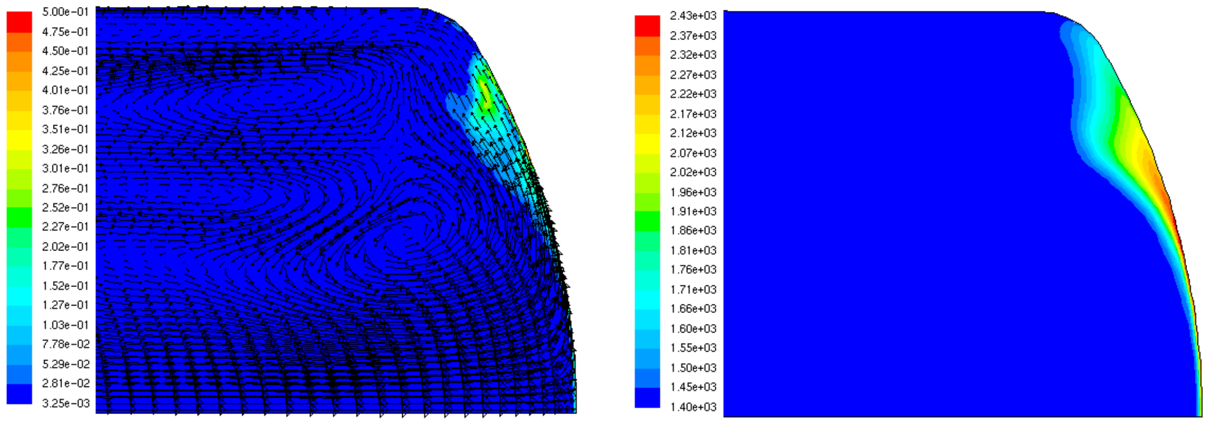


Figure 6 Computed contours of molecular viscosity and velocity vectors (left) and density (right) for model (Strata_RUN) with representation of 3-strata in the solid base layer.

DISCUSSIONS

The present study investigates the feasibility of using a Herschel-Bulkley reheology model within a single phase framework in modelling the erosion of the solid base layer. A parametric study of the Herschel-Bulkley model parameters has been carried out to assess their effects on the modelled viscosity and shear stress, thereby shedding light to establish their relative importance and influences on the rheological properties and hence the behaviour of the solid material. Amongst the four parameters examined (namely yield stress, yield viscosity, consistency factor and power-law index), it is shown that yield stress is the most influential parameter. The yield viscosity and consistency factor only have a negligible to small effect that is dependent on the range of shear rate.

The Herschel-Bulkley model was used to replicate the experimental viscosity profile of a homogenised HAL simulant suspensions at a lower solid concentration. Similarly, the Herschel-Bulkley model can be used to represent/fit the experimental viscosity profile of the actual solid base layer with higher solid concentration when data are available. The modelling would also help to identify further experiments to expand the range of viscosity data from accurate chemical simulants beyond the current operating regime.

The current approach is shown to be amenable to represent stratification in the solid layer. Initial results from a model with the representation of three generic strata are encouraging, showing the solid layer to evolve in a physically realistic manner. This extends the application envelope of the approach to represent the layering structure of the settled base layer, thereby potentially providing a powerful means to better model the complex rheological character of real solid base layers. This also highlights the additional need for rheology data of the different solid layers and their distributions.

Limitations of single phase approach with rheology model

The present approach assumes single phase flow with the solid layer at the base represented using a rheology model to treat this region as a non-Newtonian power law (Herschel-Bulkley) fluid. This offers a simple and fast (low CPU requirement) modelling technique to study the erosion dynamics of the solid base layer in response to flows in the vessel. The Herschel-Bulkley rheology model is shown to offer a viable approach to approximate the gross behaviour of the solid base layer during the initial phase of erosion. This is also supported by other detailed rheological study [3] of some natural mud-water mixtures (i.e. not too dissimilar to the solid/liquor sludge at the base) that showed the Herschel-Bulkley model to fit very well with steady flow experimental data for a large range of shear rates. This supports the use of the Herschel-Bulkley model in the current approach, and offers a convenient modeling framework for further refinements as more data (experimental and/or modelled) of the physical properties of the solid layer becomes available.

It should be noted however that this approach would not be suitable to model flows where significant interactions occur between the particulates and the primary fluid (e.g. settling of solid-liquor mixture), due to the absence of particulate representation in the model. In such circumstances a multiphase approach, such as the mixture model, would be more appropriate.

CONCLUDING REMARKS

Single phase modelling with the use of the Herschel-Bulkley model to represent the settled solid layer at the base has been used to model the erosion of the solid base layer in response to flows in an evaporator under typical operational conditions. Modelled results to date are encouraging, which show the solid base layer to evolve in a physically realistic manner.

The single phase approach using the Herschel-Bulkley model potentially offers a fast and effective modelling technique to examine the initial phase of erosion of the solid base layer. This represents a convenient modeling framework for further refinements as more data (experimental and/or modelled) of the physical properties of the solid layer becomes available.

ACKNOWLEDGEMENTS

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