

MODELING AND SIMULATION OF KRAFT TWO PHASE DIGESTER PULPING PROCESSES: MODEL DEVELOPMENT AND R&D

1 User Digester Model Setup

The user is responsible to setup the Digester Excel Spreadsheet that contains all the relevant information for the digester and that includes the setup for the parameters at the digester inlet (segment 1, west side, $i=2$ in the code). The mill provides the mass flow rate of the liquor, m_f , and the mass flow rate of the chips, m_s which is 3 times smaller than m_f . The user needs to find the density of the chips, ρ_s , and the density of the liquor, ρ_f . The liquor density can be obtained more precisely using density correlations for liquor published by TAPPI. The mill has the density ratio for that species. As of now we usually have a ratio of 1.05, $\rho_f=1000$, and $\rho_s=1050$. These values need to be improved.

The user then needs to calculate the slip velocity, s , which is the velocity ratio v_s/v_f at the inlet. This requires the user to approximate the solid fraction at the inlet, ϵ_1 (no easy method). For a hydraulic digester the flow of liquor is introduced via a high pressure line at very low solid fraction. Most of the liquor is pumped out of the top digester region via pump screens and the chips free fall through the liquor region where the solid fraction is very low. A chip level is formed where the chips continuously fall upon. The chip level changes during operation. Chip level is the major control variable in the digester. A change in level is seen by the operator as a change in the hold up of the column indicating that liquor flows need to be adjusted. Operator are concerned with chip level and chip hold up, i.e., inlet slip change and wall chip friction. We presently have problems in the model with both of these issues.

The Harkonen correlation from the Tappi paper is used to calculate the solid fraction in the digester and needs to work at the chip level location also to ensure a continuous behavior. At the chip level there is no weight of chips above, only the weight of liquor. The hydraulic pump forcing the chips and liquor slurry into the digester pressurizes the entire digester to 0.5-1.0 MPa to avoid boiling of the liquor. The pump also adds a pressure differential to the liquor for the liquor to be pushed out through all the screens and out through the bottom. The pump does not directly push the chips as there is at least a 10 m height where there is relatively no chips above the chip level. The chips move by their own weight and by the liquor flow when it moves downwards. When the liquor moves upwards, the chips weight still overcomes the liquor or else it violates continuity locally for a steady-state calculation. Only during a transient can the total chip flow be negative at a cross-section and only for a short time. As of now, we start the simulation at the chip level and ignore the conical section until the code can handle low chip solid fraction which is not the case now (long term goal). The user then needs to find the solid fraction at the top of the digester at the chip level. Here we have uncooked chips with a Kappa inlet number calculated as:

$$\text{Kappa}_{in} = \frac{100}{0.153 \frac{[Lig_{in}]}{([Lig_{in}]+[Carb_{in}]})}} \quad (1)$$

where the inlet lignin and carbohydrate concentrations at the entrance of the digester is obtained from the mill. The kappa number is in the range of 200 or more for most mills at the inlet (205 for Kamloops). Once Kappa_{in} is calculated, we need to know the solid pressure at the inlet to

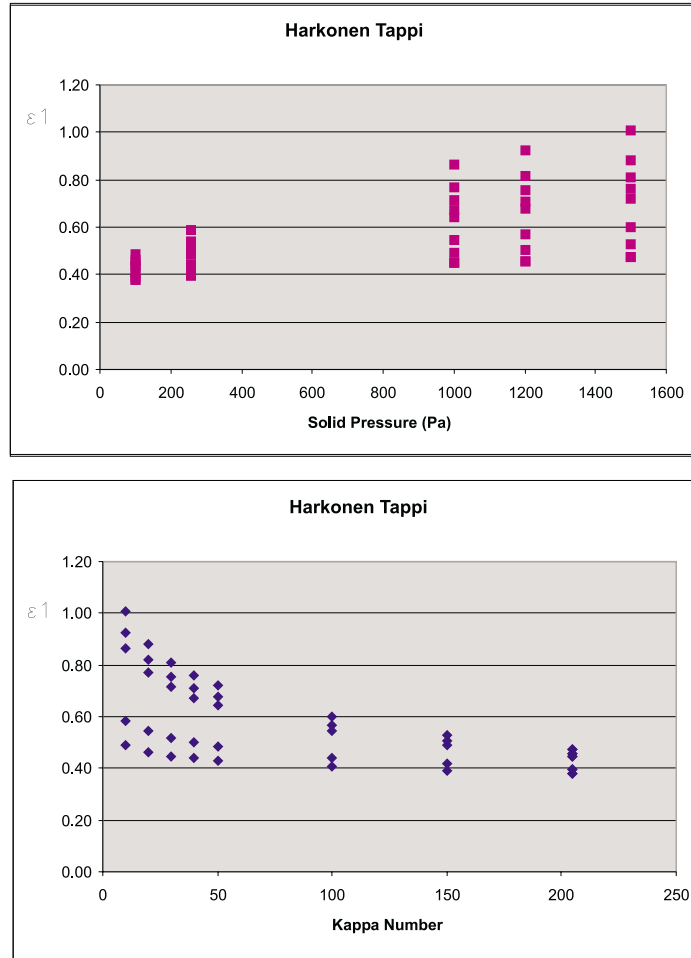


Figure 1: Harkonen Tappi correlation for solid fraction, ϵ_{1} , for different Kappa and solid pressure, P_s , values

determine the solid fraction. This is not possible to obtain so we need an approximation. Looking at Figure 1 we see that at high $Kappa_{in}$ values and low solid pressure—conditions that are occurring at the top—the solid pressure is not sensitive to both these values. Therefore we pick a value of 0.40 as most data points at low pressure converge to this value. If 0.4 does not correspond what is occurring in the real digester, then the Harkonen correlation is not applicable either. This correlations includes data taken at high Kappa and low P_s which is just uncooked chips in liquor. Note that for a digester with an IV vessel $Kappa_{in}$ will be less.

Now we take Harkonen correlation for solid fraction,

$$\epsilon_1 = 0.359 + \left(\frac{P_s}{10^4} \right)^{0.59} (0.831 - 0.139 \log k) \quad (2)$$

and determine the solid pressure at the inlet:

$$P_{s_{in}} = 10^4 \left[\frac{(\epsilon_{1_{in}} - 0.359)}{(0.831 - 0.139 \log (Kappa_{in}))} \right]^{1.695} \quad (3)$$

to make sure we will not have a discontinuity. In the code the following expression was used instead:

$$P_{sin} = 10^4 \left(\frac{\epsilon_{1in} - 0.34}{0.134} \right)^{1.695} \quad (4)$$

where it seems that the Kappa was set to 151 and the equation simplified. I am in favour of removing the above equation that occurs at many places and use the previous one. This requires the user to specify $Kappa_{in}$ which can be done in mgfd.in and ϵ_{1in} which is already an input but is overwritten in the code with a value of 0.356.

We can now calculate the inlet velocity for the liquor

$$v_{fin} = \frac{m_f}{A_{in}(1 - \epsilon_{1in})\rho_f} \quad (5)$$

where A is the area at the chip level and the slip at the inlet is:

$$s = \frac{v_{sin}}{v_{fin}} = \frac{m_s}{A\epsilon_1\rho_s v_f} = \frac{m_s(1 - \epsilon_{1in})\rho_f}{m_f(\epsilon_{1in})\rho_s} \quad (6)$$

At present the slip can be introduced directly in cmgfd.f.

```

else if (ch.eq.'v'.or.ch.eq.'w') then
  fmw(j,k)=bdat(n)*dyz
  slip = 0.387
  fmw0(j,k)=bdat(n)*dyz * slip

```

Later the slip can be entered by the user into mgfd.in.

The above slip did not work as the code was using a pressure boundary condition on the entire face of the inlet in addition to the velocity boundary condition (duplicates liquid boundary condition automatically). The pressure boundary condition causes 2 things to happen. First "npc" is set to 1 on segment 1 causing the following piece of code in subroutine line to overwrite the solid velocity at the inlet to the liquid value somehow:

```

do 7 n=1,npc
  i=ip(n)
  ns=nps(n)
  if (ns.eq.1) then
c eric -
c          up(i)=(fu(i+1)*up(i+1)-fvs(i)*vs(i)+fvn(i)*vn(i)
c      +          -fwb(i)*wb(i)
c      +          +fwt(i)*wt(i)-pr(i))/fu(i)
c eric end

```

Then the pressure boundary conditions overwrites somewhere the solid velocity imposed by the user once the above correction for up(i) is ignored. This was fixed by imposing a single pressure value, P_{sin} , at the center of the inlet.

It is important to specify all the input parameters at the inlet and make sure they do not violate the correlation. By having the user impose correct values at the inlet there should not be a discontinuity problem.

The above can work but the level correction that occurs at various places in the code that look like this:

```
cc set linear variation epsilon1
c         if(n.eq.1) then
c             if(i1+i-1.le.10) then
c                 eps1(i,j,k)=0.36
c             else if(i1+i-1.le.30) then
c                 eps1(i,j,k)=0.36+0.24*float(i1+i-1-10)/20.0
c             else if(i1+i-1.le.50) then
c                 eps1(i,j,k)=0.6-0.24*float(i1+i-1-30)/20.0
c             else
c                 eps1(i,j,k)=0.36
c             endif
c         endif
```

needs to be removed. This level correction needs to be removed as this is for a steam digester. According to Harkonen, we cannot have this low value of 0.36. I am in favour of removing this level correction everywhere in the code for the solid fraction. The solid fraction at the top should be approximately 0.4. Now we get the 0.36 value.

2 Pressure drop

The porous pressure drop across the chips is assumed to be given by

$$\alpha_{ij}(V_f - V_s) \quad (7)$$

where

$$\alpha_{ij} = \bar{\mu}^f \frac{C_f}{\Delta_f^2} \epsilon_2 \beta_{ij} \quad (8)$$

The term α_{ij} includes the influence of the chip shape and is also related to pressure drop by

$$\Delta P / \Delta l = \alpha_{ij} V \quad (9)$$

The code presently uses Harkonen correlation from his report where

$$\alpha_{ij} = 21200(\epsilon_1^2/\epsilon_2) + 9620000(\epsilon_1/\epsilon_2)V \quad (10)$$

An alternative would be to use the Tappi correlation for the pressure drop,

$$\Delta P / \Delta l = 4600(\epsilon_1/\epsilon_2)^2 V + 3900000(\epsilon_1/\epsilon_2)V^2 \quad (11)$$

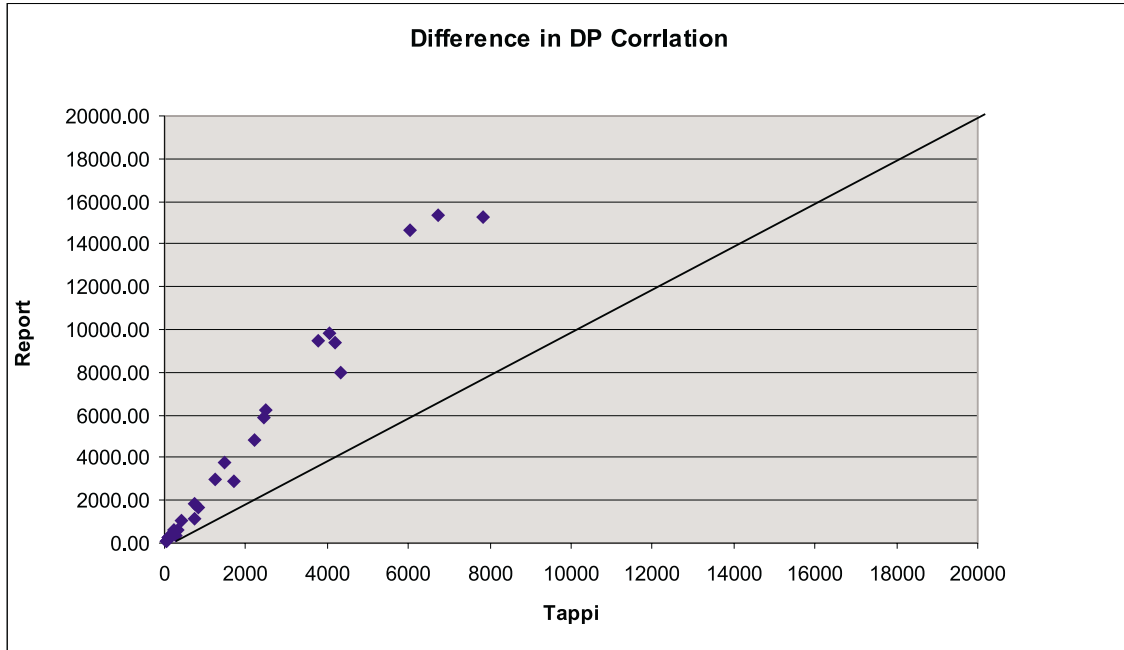


Figure 2: Harkonen Tappi Correlation for solid pressure drop versus the correlation used presently in the code from his earlier report

and deduce that (is this correct?)

$$\alpha_{ij} = 4600(\epsilon_1/\epsilon_2)^2 + 3900000(\epsilon_1/\epsilon_2)V \quad . \quad (12)$$

The difference between the 2 correlations are shown in Figure 2. There is an important difference that cannot be ignored. The current correlation for α_{ij} is **twice** the value than from what you get for the Tappi correlation. Fan can you confirm this. This could help convergence as the term $\alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s)$ is too strong.

3 Two-Phase Equations

3.1 Solid Momentum

Based on previous derivation, the solid momentum equation is:

$$\frac{D\varepsilon_1\overline{\rho_s}\overline{\mathbf{V}}_s}{Dt} = \nabla \cdot \overline{\boldsymbol{\sigma}}'_s - \varepsilon_1\nabla\overline{P}_f - \overline{\mathbf{V}}_s\dot{m}^{12} + \alpha_{ij}(\overline{\mathbf{V}}_f - \overline{\mathbf{V}}_s) + \varepsilon_1\overline{\rho_s}\mathbf{F}_s + \overline{\mu}_f\nabla^2 \cdot \mathbf{q}_s^m + \mathbf{F}_{\mu w} \quad (13)$$

Ignoring the convection term for solid, $\overline{\mu}_f\nabla^2 \cdot \mathbf{q}_s^m$, and averaging the equation we get:

$$\nabla \cdot \boldsymbol{\sigma}'_s - \varepsilon_1\nabla P_f - \mathbf{V}_s\dot{m}^{12} + \alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s) + \varepsilon_1\rho_s\mathbf{F}_s + \mathbf{F}_{\mu w} = 0 \quad (14)$$

Now separate the stress tensor into the solid pressure and the apparent solid viscosity, we get:

$$\nabla \cdot \boldsymbol{\sigma}'_s = -\nabla P_s + \nabla \cdot \mu_s\nabla\mathbf{V}_s \quad (15)$$

The chip shear stress is modeled as an apparent viscosity as an approximation to account for the dissipation forces when the chips shear against each other. The chips have a high propensity not to move relative to each other. Therefore the apparent viscosity is large. The rheological law of chips can be compared to the rheology of a viscous-plastic fluid which is shown in Figure 3a. There is a region where a shear stress produces no strain in the fluid. When the yield stress is exceeded, the stress varies linearly with the strain and a constant viscosity can be assumed. It is difficult to postulate a constant viscosity for chips as the shear force value will be influenced by the normal force (solid pressure), the kappa number, and the chip length to width dimensions which vary throughout the digester. It may therefore not be correct to assume a constant μ_s to predict the solid shear. The rheology of chips may in fact be more complicated and behave more like high consistency fibers. At high consistency, pressing on the fiber mixture will cause the force to be transmitted across the fiber matrix, giving rise to a solid pressure like wood chips in a digester. For fibers, the length to width ratio is critical as they form a network causing a rheology shown in Figure 3b. For $\tau < \tau_{yield}$, there is no strain rate. Afterwards, two regimes can be identified. For τ less than the fiber network disruptive stress, τ_d , the flow is non-newtonian and the flow is assumed laminar. When the network is broken, $\tau > \tau_d$, the flow can be assumed turbulent. In this region there is no fiber network. Chips will not follow the same rheology as fibers as they do not possess the ability to form networks but can interfere with each other due to the chip shape which is elongated making them form a sort of "interlock". They do however have friction forces and the ability to transfer normal forces. Like fibers, chips can have discontinuities which can be referred to as "channeling". A column of chips may be stagnant in one area while another area may be moving more freely. The discontinuity is not unlike a fiber matrix where there is turbulent fiber network structure that is broken, a laminar region, and a stagnant region.

Combining the above two equations and defining the body force as gravity we get: where

$$-\underbrace{\nabla \cdot \mu_s\nabla\mathbf{V}_s}_{\mathbf{I}^1} = -\underbrace{\nabla P_s}_{\mathbf{I}^2} - \underbrace{\varepsilon_1\nabla P_f}_{\mathbf{I}^3} - \underbrace{\mathbf{V}_s\dot{m}^{12}}_{\mathbf{I}^4} + \underbrace{\alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s)}_{\mathbf{I}^5} - \underbrace{\varepsilon_1\rho_s g \nabla \cdot \mathbf{z}}_{\mathbf{I}^6} + \underbrace{\mathbf{F}_{\mu w}}_{\mathbf{I}^7} \quad (16)$$

- I_1 solid shear stress term modelled as an apparent viscosity;

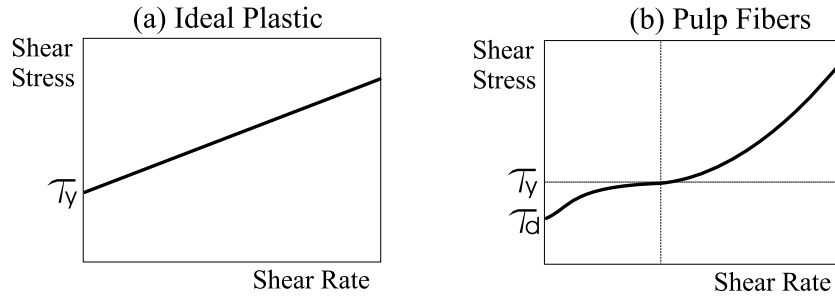


Figure 3: Stress-Strain relationship for (a) ideal plastic, and (b) pulp slurry

- I_2 solid pressure due to the normal force the chips exert onto each other as soon as they form a matrix structure;
- I_3 component of fluid pressure transferred from the liquid to the chips (any change in dynamic velocity will result in a pressure force on the chips);
- I_4 force arising from the mass exchange occurring during delignification;
- I_5 frictional force between fluid and chips when phases travel at different velocities in the element of volume (note that a zero slip is assumed between liquid and chips within the element of volume);
- I_6 the body force from gravity, and
- I_7 the wall friction force at the wall between the chip phase and the wall (force holding the chip column in the digester).

In the present code, $F_{\mu w}$, the wall friction force between the shell and the chips is set to zero and modeled as a wall model. Using the solid apparent viscosity to model this wall friction force is hard to physically justify as interlocking of chips do not occur. This is apparent in the result which show a very large velocity profile for the chips, as shown in Figure 4. It is known that the chips travel more as a plug. It is also very reasonable to assume that it is easier for chips to rub against the wall than against each other. The code will have to be modified to model the sliding friction between the chips and the wall, as this is a very important parameter.

The large chip velocity profile maybe caused by the wall shear stress for the solid equation is much to strong compared to the internal shear stress in the solid phase resulting in an artificial velocity profile. By relieving the wall shear stress, it is hoped that the profile will ease up.

Direct experimental evidence that chips travel as a plug is hard to find but is available. The radio active tracers showed this in 1960. Some evidence also comes from digesters that go through a hardwood/softwood grade change. The mixing region between the 2 different layers is less than 10 feet when it come out of the digester. Our results would show that the chips mixed layer would be significantly larger. The mixing layer is seen by the color change. When the mill stops pouring hardwood into the chip bin which is of a certain color and start pouring softwood chips of a different color, a chip layer transition of different colors is formed. As the initial horizontal transition zone proceeds down the 40 m chip bin some mixing occurs. The chips are then fed into the impregnation vessel where further mixing occurs as purely plug flow is not possible. The

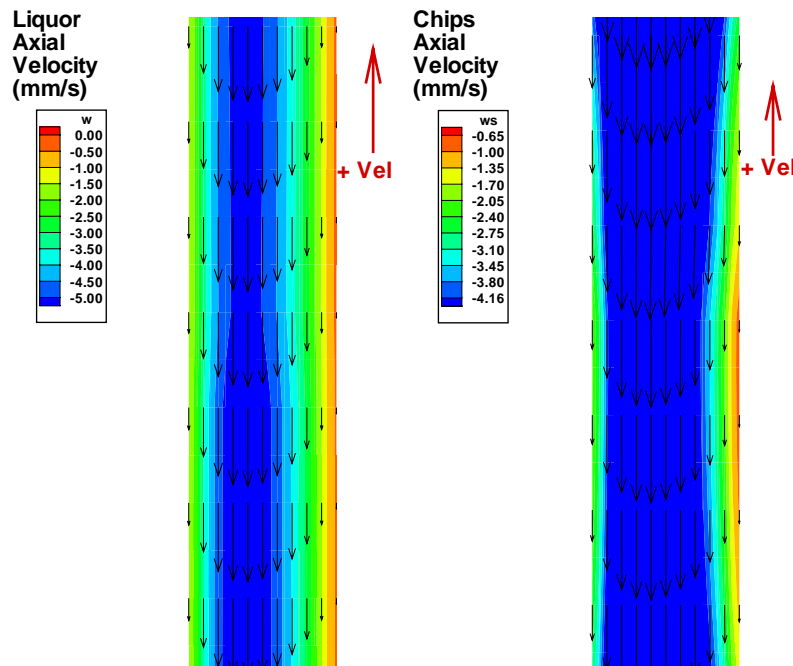


Figure 4: Fluid and chips velocity profiles as per model digester model

hardwood/softwood chip interface then proceeds into the main digester where it flows almost as a plug flow and exits. When the chips finally exit the digester, the mill reports less than 10 feet of transition zone for softwood and hardwood from the color transition of the fibers. A significant portion of that 10 feet is due to the mixing occurring in the chip bin and impregnation vessel. So the digester may account for less than 5 feet of this transition which requires chips to move almost as a plug. The results shown in Figure 4 where the chips travel 3-4 times faster in the middle would produce a thick mixed zone. Therefore it is hard to believe strong chip velocity profiles and chips flowing upwards. When the liquor flows upward it is typically in the 1 – 3 mm/s range. This liquor velocity translates to app 5 minutes to move 1 meter. The chip upward flow is app 10 m giving 50 minute for the liquor to move through that space. This does not translate to a large force to push chips upwards as the shear forces between the chips are very large. Unless the solid pressure is very small due to dilution, it is very hard to move chips upwards in the digester and the flows that we deal with are not strong enough to do this (except near downcomers).

The pronounce laminar liquor profile is also not correct. If the liquor flows much faster in the center, we expect that the differential velocity will be much greater in the center (once chips flow more like a plug). This will lead to a local fluid pressure increase as the dynamic velocity converts into fluid pressure. A local increase in pressure in the middle must translate into a radial fluid motion, thus reducing the liquor flow profile.

The first step to solve this problem is to fix the code so that the solid equation predicts the velocity that one would obtain by simple continuity. It may be worth while at this stage to also write the solid velocity at the end of an iteration by performing a simple continuity equation by taking into account the inlet solid velocity and the solid fraction and assume plug flow to compare to what the code predicts.

The second step is to remove the wall shear stress for the solid phase and impose a sliding friction

as a boundary condition in the code. This would be done by forcing all faces except at the top and bottom to be a sliding friction, even at the screens. Sliding friction is caused by friction between the wall and the moving solid particles. The chips sliding force has a magnitude that is proportional to the normal force N pressing against the wall and can be approximated by:

$$d\mathbf{F}_{\mu w} = \mu_{fr}\mathbf{N} = \mu_{fr}\overline{P_s} dA = \mu_{fr}P_s \pi d \varepsilon_1 A_c \delta l \quad (17)$$

where the solid surface contact is assumed to be related to the solid fraction, and only a portion of the solid fraction is in actual contact with the vessel. The contact area factor, A_c , needs to be obtained experimentally. The Pulp and Paper Center is willing to do this. The frictional force as a volume force can be written as:

$$\mathbf{F}_{\mu w} = \frac{d\mathbf{F}_{\mu w}}{dV} = \frac{\mu_{fr}\overline{P_s}\pi d\varepsilon_1 A_c \delta l}{\frac{1}{4}\pi d^2\delta l} = \frac{4\mu_{fr}P_s \varepsilon_1 A_c}{d} \quad (18)$$

Alternatively, the frictional force can be seen as an average coefficient averaged over the chip area and the force becomes:

$$\mathbf{F}_{\mu w} = \frac{4\mu_{fr_{avg}}P_s \varepsilon_1}{d} \quad (19)$$

Thus the solid momentum equation is:

$$-\nabla \cdot \mu_s \nabla \mathbf{V}_s = -\nabla P_s - \varepsilon_1 \nabla P_f - \mathbf{V}_s \dot{m}^{12} + \alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s) - \varepsilon_1 \rho_s g \nabla \cdot \mathbf{z} + \mathbf{F}_{\mu w} \quad (20)$$

3.2 Liquid Momentum

Based on previous derivation, the liquid momentum equation is:

$$\frac{D\varepsilon_2\overline{\rho_f}\overline{\mathbf{V}_f}}{Dt} = \nabla \cdot \mu_f \nabla \overline{\mathbf{V}_f} - \alpha_{ij}(\overline{\mathbf{V}_f} - \overline{\mathbf{V}_s}) - \varepsilon_2 \nabla \overline{P_f} + \overline{\mathbf{V}_s} \dot{m}^{12} + \varepsilon_2 \overline{\rho_f} \mathbf{F}_f \quad (21)$$

For steady-state, imposing the gravity, and rearranging we get:

$$\underbrace{\mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f)}_{\mathbf{I}^1} - \underbrace{\nabla \cdot \mu_f \nabla \mathbf{V}_f}_{\mathbf{I}^2} = - \underbrace{\varepsilon_2 \nabla P_f}_{\mathbf{I}^3} - \underbrace{\alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s)}_{\mathbf{I}^4} + \underbrace{\mathbf{V}_s \dot{m}^{12}}_{\mathbf{I}^5} - \underbrace{\varepsilon_2 \rho_f g \nabla \cdot \mathbf{z}}_{\mathbf{I}^6} \quad (22)$$

where

- I_1 momentum of fluid;
- I_2 liquid viscosity term;
- I_3 fluid pressure;
- I_4 frictional force between fluid and chips when phases travel at different velocities in the element of volume
- I_5 force arising from the mass exchange occurring during delignification, and

- I_6 the body force from gravity.

The terms $\varepsilon_2 \nabla P_f$ and $\alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s)$ are large. The first attempt was to solve a separate solid pressure equation. This was abandoned and is no longer used. Instead the solid and momentum equations (Equations 16 and 22) are combined as follows:

$$\begin{aligned} \mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f) - (\nabla \cdot \mu_f \nabla \mathbf{V}_f + \nabla \cdot \mu_s \nabla \mathbf{V}_s) = \\ -\nabla P_s - \varepsilon_1 \nabla P_f - \varepsilon_2 \nabla P_f - \varepsilon_2 \rho_f g \nabla \cdot \mathbf{z} - \varepsilon_1 \rho_s g \nabla \cdot \mathbf{z} + \mathbf{F}_{\mu w} \end{aligned} \quad (23)$$

giving

$$\begin{aligned} \mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f) - (\nabla \cdot \mu_f \nabla \mathbf{V}_f + \nabla \cdot \mu_s \nabla \mathbf{V}_s) = \\ -\nabla(P_s + P_f) - \varepsilon_2 \rho_f g \nabla \cdot \mathbf{z} - \varepsilon_1 \rho_s g \nabla \cdot \mathbf{z} + \mathbf{F}_{\mu w} \end{aligned} \quad (24)$$

Now the solid velocity can be written as:

$$\begin{aligned} \mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f) - (\nabla \cdot \mu_f \nabla \mathbf{V}_f + \nabla \cdot \mu_s \nabla (\mathbf{V}_s + \mathbf{V}_f - \mathbf{V}_f)) = \\ -\nabla(P_s + P_f) - \varepsilon_2 \rho_f g \nabla \cdot \mathbf{z} - \varepsilon_1 \rho_s g \nabla \cdot \mathbf{z} + \mathbf{F}_{\mu w} \end{aligned} \quad (25)$$

leaving

$$\begin{aligned} \mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f) - \nabla \cdot (\mu_f + \mu_s) \nabla \mathbf{V}_f = \\ \nabla \cdot \mu_s \nabla (\mathbf{V}_s - \mathbf{V}_f) - \nabla(P_s + P_f) - \varepsilon_2 \rho_f g \nabla \cdot \mathbf{z} - \varepsilon_1 \rho_s g \nabla \cdot \mathbf{z} + \mathbf{F}_{\mu w} \end{aligned} \quad (26)$$

This is the liquid equation which needs to be solved. The liquid and solid viscosities have been combined as well as the pressures. You can assume $\mu_f \ll \mu_s$. Now we assume the liquid pressure $P' = P_f + P_s$. The boundary conditions are still for liquid velocities. We assume only laminar flow.

Rewriting we get

$$\begin{aligned} \mathbf{V}_f \nabla \cdot (\varepsilon_2 \rho_f \mathbf{V}_f) - \nabla \cdot \mu_s \nabla \mathbf{V}_f = \\ -\nabla P'_f + \nabla \cdot \mu_s \nabla (\mathbf{V}_s - \mathbf{V}_l) - \varepsilon_2 \rho_f \mathbf{F}_f - \varepsilon_1 \rho_s \mathbf{F}_s + \mathbf{F}_{\mu w} \end{aligned} \quad (27)$$

The solid equation can be rewritten by taking into account that

$$-\nabla P_s - \varepsilon_1 \nabla P_f = -\varepsilon_2 \nabla P_s - \varepsilon_1 \nabla P' \quad (28)$$

so that the solid equation becomes:

$$-\nabla \cdot \mu_s \nabla \mathbf{V}_s = -\varepsilon_2 \nabla P_s - \varepsilon_1 \nabla P' - \mathbf{V}_s \dot{m}^{12} + \alpha_{ij}(\mathbf{V}_f - \mathbf{V}_s) + \varepsilon_1 \rho_s \mathbf{F}_s + \mathbf{F}_{\mu w} \quad (29)$$

The program solves for P'_f , not P_f for liquid and solid.

According to the conservation law, the mass conservation for liquid can be written as:

$$\nabla \cdot \varepsilon_2 \rho_f \mathbf{V}_f + \nabla \cdot \varepsilon_1 \varepsilon_{12} \rho_f \mathbf{V}_s - \dot{m}^{12} = 0 \quad (30)$$

or

$$\nabla \cdot \varepsilon_2 \rho_f \mathbf{V}_f = \dot{m}^{12} - \nabla \cdot \varepsilon_1 \varepsilon_{12} \rho_f \mathbf{V}_s \quad (31)$$

The term $\dot{m}^{12} - \nabla \cdot \varepsilon_1 \varepsilon_{12} \rho_f \mathbf{V}_s$ is programmed as the variable $\text{pls}(i,j,k)$ in the program for the liquid equation.

The solid continuity equation is:

$$\nabla \cdot \varepsilon_1 \varepsilon_{11} \rho_s \mathbf{V}_f + \dot{m}^{12} = 0 \quad (32)$$

From Equation 29 we get

$$(\dot{m}^{12} + \alpha_{ij}) \mathbf{V}_s = -\varepsilon_2 \nabla P_s - \varepsilon_1 \nabla P'_f + \varepsilon_1 \rho_s \mathbf{F}_s + \alpha_{ij} \mathbf{V}_f + \nabla \mu_s \nabla \mathbf{V}_s \quad (33)$$

and solving for \mathbf{V}_s we get:

$$\mathbf{V}_s = \frac{\alpha_{ij}}{(\dot{m}^{12} + \alpha_{ij})} \mathbf{V}_f - \frac{\varepsilon_2}{(\dot{m}^{12} + \alpha_{ij})} \nabla P_s - \frac{\varepsilon_1}{(\dot{m}^{12} + \alpha_{ij})} \nabla P'_f + \frac{1}{(\dot{m}^{12} + \alpha_{ij})} \nabla \cdot \mu_s \nabla \mathbf{V}_s + \frac{1}{(\dot{m}^{12} + \alpha_{ij})} (\varepsilon_1 \rho_s \mathbf{F}_s) \quad (34)$$

Combining above 2 equations we get:

$$\begin{aligned} \nabla \cdot \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})} \varepsilon_2 \nabla P_s = \\ -\nabla \cdot \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})} \varepsilon_1 \nabla P'_f + \nabla \cdot \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})} \alpha \mathbf{V}_f + \nabla \cdot \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})} \nabla \cdot \mu_s \nabla \mathbf{V}_s + \nabla \cdot \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})} \mathbf{F}_s \end{aligned} \quad (35)$$

Equation 35 is the solid pressure equation solved implicitly by the line solver. Now setting $\beta(i, j, k)$ in the code to $\beta = \frac{\varepsilon_1 \varepsilon_{11} \rho_s}{(\dot{m}^{12} + \alpha_{ij})}$ we get:

$$\nabla \cdot \beta \varepsilon_2 \nabla P_s = -\nabla \cdot \varepsilon_1 \beta \nabla P'_f + \nabla \cdot \beta \nabla \mu_s \nabla \mathbf{V}_s + \nabla \cdot \beta \mathbf{F}_s \quad (36)$$

Note: According to Pingfan the mass transfer term is still set to zero (something like ε_{11}) still zero and was never tested.

4 List of things to fix

- Must be able to have slip velocity at inlet and have a reasonable converged solution. We have not been able to do this.
- Need wall friction model independent of large viscosity
- Need to remove level model at inlet.
- Must be able to predict plug profile or almost plug profile of chips. At present I do not believe the large solid velocity profile.
- The flow velocity needs to react to the plug flow chip profile and readjust accordingly
- Need to go back to delignification model and model [S]

5 Nomenclature

Symbol	Description
A	Area
c_α	Specific heat capacity of phase α
C_f	A macroscopic dimensionless shape factor
d	Diameter
d_p	Pore diameter
e	Void ratio ($= U_{ou}/U_{os}$). Density of an extensive quantity, E
E	Young's modulus of elasticity
E_α	Specific energy for the α -phase
f	Subscript denoting free liquor
F_Λ	Force of dry friction
F_μ	Interphase friction force
g	Acceleration due to gravity
G_{ijk}	Tensorial quantity
h	Specific enthalpy
\mathbf{I}	Unit tensor
\mathbf{J}^{EV}	Diffusive flux of E
k_{sf}	Heat transfer coefficient between chip and liquid
$k_{\alpha w}$	Heat transfer coefficient between α -phase and wall
l	Length
m	Mass
\dot{m}^{12}	Mass transfer between phases s and f
M_{air}	Molar weight of air
M_{water}	Molar weight of water
ns	Subscript denoting insoluble material in a chip
N	Normal force
$[OH]$	Effective alkali concentration
P_α	Pressure for α -phase
Q_{sz}	Vertical heat of conduction in chips
Q_{slw}	Sum of inter-phase heat of conduction and that through the side walls
R	Molar gas constant
R_{lig}	Reaction rate of lignin
R_{carb}	Reaction rate of carbohydrates
$[S]$	Effective sulfide
t	Time coordinate

T_α	Phase temperature
T_w	Wall temperature
\mathbf{u}_α	Velocity at which the S_{sf} surface is being displaced
U_i	Specific internal energy
U	Volume
U_0	Volume of domain
\mathbf{v}_α	Average velocity of α -Phase
V^E	Averaged E velocity
\mathbf{V}_α	Phase velocity
x_i	Rectangular coordinates, $i=1, 2, \text{ or } 3$
α	α -phase, $\alpha=f, s$
α_{ij}	Flow resistance tensor
α_{lig}	Content of lignin in a wood chip
α_{carb}	Content of carbohydrate in a wood chip
α_{sul}	Content of sulfide
β	β -phase
Γ^E	Rate of production of E per unit mass of phase
Δ	Characteristic distance from solid surface to fluid within void space
Δ_{alpha}	Hydraulic radius of α -phase
Δh_r	Heat of reaction
ε_α	Volume fraction of α -phase
ε_{11}	Volume fraction of wood material in a chip
ε_{12}	Volume fraction of liquid in a chip
∇	Divergence operator
κ	Kappa number
λ	Specific latent heat of condensation
λ_α	Thermal conductivity of α -phase
λ_w	Latent heat of vaporization of water
μ_α	Dynamic viscosity of α -phase
ρ_α	Mass density of α -phase
σ	Stress tensor
$\Sigma_{\alpha\beta}$	Specific area of $S_{\alpha\beta}$. Similarly, $\Sigma_{\alpha\alpha}$, etc.
τ	The sum of R_{lin} and R_{carb}
ν	Normal unit vector on S_{sf} outward to the α -phase
φ_E	Flux of energy at the boundary
Φ	Specific potential energy