Introducing non-Newtonian fluid mechanics computations with *Mathematica*® in the undergraduate curriculum

Housam BINOUS*

National Institute of Applied Sciences and Technology

BP 676 Centre Urbain Nord, 1080 Tunis, Tunisia

***corresponding author:** binoushousam@yahoo.com

Bibliographical Sketch of Author

Dr. Housam BINOUS is a full time faculty member at the National Institute of Applied Sciences and Technology in Tunis. He earned a Diplôme d'ingénieur in biotechnology from the Ecole des Mines de Paris and a Ph.D. in chemical engineering from the University of California at Davis. His research interests include the applications of computers in chemical engineering.

Abstract

We study four non-Newtonian fluid mechanics problems using *Mathematica*®. Constitutive equations describing the behavior of power-law, Bingham and Carreau models are recalled. The velocity profile is obtained for the horizontal flow of power-law fluids in pipes and annuli. For the vertical laminar film flow of a Bingham fluid we determine the velocity profile. Both problems involve the use of the shooting techniques because they have split boundary conditions. Since *Mathematica*® permits symbolic computations, we determine analytical expressions of volumetric flow rates for pipe flow of the Bingham and power-law fluids. We use the built-in optimization command of *Mathematica*®, *FindMinimum*, in order to find the non-Newtonian fluid model from representative data of flow rates measured under different applied pressure gradients in a horizontal pipe. These pedagogic problems are used to introduce the field of non-Newtonian fluid mechanics to students at the National Institute of Applied Sciences in Tunis. The *Mathematica*® notebooks are available from the corresponding author upon request or at Wolfram Research[1].

Keywords: Carreau, power-law and Bingham fluids, annulus and pipe flow

A non-Newtonian fluid has a viscosity that changes with the applied shear force. These fluids are characterized by measuring or computing several rheological properties such as the viscosity and the first and second normal stresses. Rheometers are used, under oscillatory shear flow or extensional flow, to obtain experimental values of these rheological properties while kinetic theory calculations using dumbbells allow the prediction of these rheological properties. For a Newtonian fluid (such as water), the viscosity is independent of how fast you are stirring it, but for a non-Newtonian fluid it is dependent. It gets easier or harder to stir faster for different types of non-Newtonian fluids. By adding corn starch to water, one obtains a non-Newtonian fluid. Applying agitation with a spoon makes the fluid behave like a solid. Thus, the shear-thickening property of this non-Newtonian fluid becomes apparent. When agitation is stopped and the fluid is allowed to rest for a certain period of time, it recovers its liquid-like behavior.

Many peculiar phenomena are observed with non-Newtonian fluids and constitute "fun" experiments that students can perform in the laboratory. They include dye swelling and rod climbing as well as the behavior of suspensions of particles moving in non-Newtonian versus Newtonian fluids. Students can determine the terminal fall velocity and rotation direction of a single settling particle as well as wall effects and interaction between particles. Problems involving non-Newtonian fluid flow are ubiquitous in modern industry, such as in polymer processing plants. The study of body fluids such as blood, which are non-Newtonian, has important applications in biomedical engineering. In the present paper, we show how one can use the mathematical software, *Mathematica*®, to solve some simple non-Newtonian fluid problems. The most relevant *Mathematica*® commands are inserted in the text and can be found in the any introductory book such as *Mathematica® , A System for doing Mathematics by Computer* by Stephen Wolfram[2]. We start by reminding the reader of the few simple constitutive equations for the power-law, Carreau and Bingham fluids. Then, we give the velocity profile for the horizontal flow of power-law and Carreau fluids in a pipe and an annulus. The velocity profile for the fall of a Bingham liquid film is obtained in the next section. We also derive volumetric flow rate expressions for pipe flow of Bingham and power-law fluids. In the last part of the paper, we make a model determination using the previously found volumetric flow rate expressions and representative data.

I- Constitutive equations for non-Newtonian fluids

For Newtonian fluids, the shear stress, τ , is proportional to the strain rate, $\dot{\gamma}$

$$\tau = \eta \dot{\gamma} \tag{1}$$

where the viscosity, η, the proportionality factor, is constant. The situation is different for non-Newtonian fluids and the viscosity is a function of the strain rate:

$$\tau = \eta\left(\dot{\gamma}\right)\dot{\gamma} \tag{2}$$

Different constitutive equations, giving rise to various models of non-Newtonian fluids, have been proposed in order to express the viscosity as a function of the strain rate.

In power-law fluids, the following relation is satisfied:

$$\eta = \kappa \dot{\gamma}^{n-1} \tag{3}$$

Dilatant fluids correspond to the case where the exponent in equation (3) is positive ($n > 1$) while pseudo-plastic fluids are obtained when $n < 1$. We see that viscosity decreases with strain rate for $n < 1$, which is the case for pseudo-plastic fluids, also called shear-thinning fluids. On the other hand, dilatant fluids are shear-thickening. If $n = 1$, one recovers the Newtonian fluid behavior.

The Carreau model describes fluids for which the viscosity presents a plateau at low and high shear rates separated by a shear-thinning region:

$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = \frac{1}{\left[1 + (\lambda \dot{\gamma})^2\right]^{(1-n)/2}} \tag{4}$$

where η_0 is the zero-shear viscosity and η_∞ is the infinite-shear viscosity.

Finally, the Bingham model is defined as follows:

$$\text{At low shear rates:} \quad \frac{1}{2}(\tau : \tau) \le \tau_0^2, \qquad \dot{\gamma} = 0 \tag{5}$$

$$\text{At high shear rates:} \quad \frac{1}{2}(\tau : \tau) > \tau_0^2, \qquad \tau = \left(\eta + \frac{\tau_0}{\dot{\gamma}}\right)\dot{\gamma} \tag{6}$$

II. Horizontal Flow of Carreau and Power-Law Fluids in a Pipe

Problem statement. Find the velocity profiles for the laminar flow of power-law and Carreau fluids in a pipe, shown in Fig. 1. Use the following values for the pressure difference Δ*p*, the exponent *n*, the Newtonian fluid viscosity η, the consistency index *κ*, the infinite-shear viscosity η_∞, the zero-shear viscosity η_0, the relaxation parameter λ, the pipe length *L* and radius *R*, whose units appear under "Nomenclature" at the end of this article:

$$\Delta P = 100; \quad L = 50 \quad \text{and} \quad R = 0.02$$

Newtonian fluid: $\eta = 8.9 \text{ x}10^{-4}$.

Dilatant fluid: $n = 3.39$ and $\kappa = 10^{-6}$.

Pseudo-plastic fluid: $n = 0.4$ and $\kappa = 5 \text{ x}10^{-3}$.

Carreau fluid: $n = 0.5$, $\lambda = 0.2$, $\eta_0 = 1.72 \text{ x}10^{-3}$ and $\eta_\infty = 0$.

Solution. This problem is treated using Polymath©, a numerical computational package[3], in the *Problem Solving in Chemical Engineering with Numerical Methods* by Cutlip and Shacham[4]. The governing equation is the z-component of the equation of motion in cylindrical coordinates:

$$\frac{1}{r}\frac{d}{dr}\left[r\kappa\left(-\frac{dv_z}{dr}\right)^n\right] = \frac{\Delta P}{L} \tag{7}$$

Equation (7) is subject to the following split boundary conditions:

$$\text{At} \quad r = 0: \qquad \tau_{rz} = 0 \tag{8}$$

$$\text{At} \quad r = R: \qquad v_z = 0 \tag{9}$$

These kinds of mathematical problems often require the utilization of a particular numerical approach called the shooting technique. This method consists of guessing different values of v_z at $r = 0$, solving the differential equation and checking that the no-slip boundary condition at $r = R$ is satisfied. An analytical solution is possible for power-law fluids and details about its derivation can be found in *Fluid Mechanics for Chemical Engineers* by Wilkes[5]:

$$v_z(r) = \left(\frac{\Delta P}{L}\frac{1}{2\kappa}\right)^{1/n} \frac{\left(R^{1+1/n} - r^{1+1/n}\right)}{\frac{1}{n}+1} \tag{10}$$

For the Carreau fluid, one must use a numerical approach since no analytical solution is available.

For the power-law fluids, the following *Mathematica*® commands are used to find the velocity:

```
system[Ω_] = {D[r τrz[r], {r, 1}] == ΔP / L r,
   D[vz[r], {r, 1}] == If[τrz[r] ≥ 0, - (τrz[r] / κ)^(1 / n),
     (-τrz[r] / κ)^(1 / n)], τrz[10^-5] == 0, vz[10^-5] == Ω};
myODEsoln[Ω_] := NDSolve[system[Ω], {vz, τrz}, {r, 10^-5, R}]
yend[Ω_?NumericQ] := Flatten[(vz[r] /. myODEsoln[Ω]) /. r → R]
bc = FindRoot[yend[Ω] == 0, {Ω, 0, 0.5}][[1, 2]];
```

The graphical capability of *Mathematica*® allows the student to plot the velocity profile without having to use different software. Figure 2 shows the velocity profile for the Newtonian, dilatant, Carreau and pseudo-plastic cases using the commands:

```
sol1 = myODEsoln[bc]
plt1 = Plot[vz[r] /. sol1, {r, 0.00001, R}, PlotStyle → RGBColor[0, 0, 1]]
```

These profiles are obtained under the equal volumetric flow conditions. The velocity near the wall is higher for the Carreau and pseudo-plastic fluids than for the Newtonian and dilatant fluids. This results in higher heat transfer rates due a higher convection. The author's opinion is that the approach to solve split boundary problems using *Mathematica*® is more systematic than the one proposed by Cutlip and Shacham[4] using Polymath© despite a steeper initial learning curve for the students. In fact, it automatically finds the velocity at the center of the pipe by verifying the no-slip boundary condition and using the *Mathematica*® command FindRoot.

II. Horizontal Flow of a Carreau and a Power-Law Fluid in an annulus

Problem statement. Find the velocity profiles for the laminar flow of a power-law and Carreau fluids in an annulus, shown in Fig. 3. Use the following values, where R_1 and R_2 are the inner and outer radii, and all other symbols have already been defined:

$$\Delta P = 100; \quad L = 50; \quad R_1 = 0.02 \quad \text{and} \quad R_2 = 0.05$$

Newtonian fluid: $\eta = 8.9 \times 10^{-4}$.

Dilatant fluid: $n = 1.2$ and $\kappa = 4.7 \times 10^{-4}$.

Pseudo-plastic fluid: $n = 0.5$ and $\kappa = 4.5 \times 10^{-3}$.

Carreau fluid: $n = 0.5$, $\lambda = 0.2$, $\eta_0 = 2.04 \times 10^{-3}$ and $\eta_\infty = 0$.

Solution. Cutlip and Shacham[4] have solved this example using Polymath©. The governing equation is again the z-component of the equation of motion in cylindrical coordinates:

$$\frac{1}{r}\frac{d}{dr}\left[r\kappa\left(-\frac{dv_z}{dr}\right)^n\right] = \frac{\Delta P}{L} \tag{11}$$

Equation (11) is subject to the following split boundary conditions:

$$\text{At} \quad r = R_1: \qquad v_z = 0 \tag{12}$$

$$\text{At} \quad r = R_2: \qquad v_z = 0 \tag{13}$$

To solve this problem, we make use of the shooting technique in a similar fashion as the previous example. This method consists of guessing different values of τ_{rz} at $r = R_1$, solving the differential equation and checking that the no-slip boundary condition at $r = R_2$ is satisfied. An analytical solution[4] is available for the Newtonian fluid case:

$$v_z(r) = \left(\frac{\Delta P}{4\eta L}\right)\left[R_2^2 - r^2 + \frac{R_2^2 - R_1^2}{\ln(R_2/R_1)}\ln(r/R_2)\right] \tag{14}$$

No analytical solution is available for dilatant, pseudo-plastic and Carreau fluids and one must resort to a numerical method.

For the power-law fluids, the following *Mathematica*® command is used to find the velocity as a function of r:

```
system[Ω_] = {D[r τrz[r], {r, 1}] == ΔP / L r,
   D[vx[r], {r, 1}] == If[τrz[r] ≥ 0, -(τrz[r] / κ)^(1/n), (-τrz[r] / κ)^(1/n)],
   τrz[R1] == Ω, vz[R1] == 0};
myODEsoln[Ω_] := NDSolve[system[Ω], {vz, τrz}, {r, R1, R2}]
yend[Ω_?NumericQ] := Flatten[(vz[r] /. myODEsoln[Ω]) /. r → R2]
bc = FindRoot[yend[Ω] == 0, {Ω, -2, 2}][[1, 2]];
```

One can plot the velocity profile, shown in Figure 4, for the Newtonian, dilatant, Carreau and pseudo-plastic cases using the *Mathematica*® commands:

```
sol1 = myODEsoln[bc]
plt1 = Plot[vx[r] /. sol1, {r, 0.00001, R}, PlotStyle → RGBColor[0, 0, 1]]
```

These profiles are obtained under equal volumetric flow conditions. The velocity profiles found, for all four fluids, are not symmetric. In fact, they reach a maximum value close to the radial position given by $r = 0.033$, slightly less than half-way from R_1 and R_2.

IV- Vertical laminar flow of a Bingham liquid film

Problem statement. Find the velocity profile for the vertical laminar flow of a Bingham fluid down the wall depicted in Figure 5. Values of the gravitational acceleration, g, the density, ρ, the yield stress, τ_0, the zero-shear viscosity, η_0, the film thickness, δ, are given by:

$$g = 9.81; \quad \rho = 950; \quad \tau_0 = 5; \quad \eta_0 = 0.15 \quad \text{and} \quad \delta = 0.005$$

Solution. Cutlip and Shacham[4] have presented a solution of this example using Polymath©. The governing equation is the z-component of the equation of motion in rectangular coordinates:

$$\frac{d\tau_{xz}}{dx} = \rho g \tag{15}$$

Equation (15) is subject to the following split boundary conditions:

$$\text{At} \quad x = 0: \qquad \tau_{xz} = 0 \tag{16}$$

$$\text{At} \quad x = \delta: \qquad v_z = 0 \tag{17}$$

We make the same treatment as the first two problems by applying the shooting technique:

```
system[Ω_] = {D[τxz[x], {x, 1}] == ρ g,
   D[vz[x], {x, 1}] == If[Abs[τxz[x]] ≤ τ0, 0,
     If[τxz[x] > τ0, (τ0 - τxz[x]) / η0, -(τ0 + τxz[x]) / η0]], τxz[0] == 0, vz[0] == Ω};
myODEsoln[Ω_] := NDSolve[system[Ω], {vz, τxz}, {x, 0, δ}]
yend[Ω_?NumericQ] := Flatten[(vz[r] /. myODEsoln[Ω]) /. r → δ]
bc = FindRoot[yend[Ω] == 0, {Ω, 0, 0.5}][[1, 2]];
```

For the Newtonian case, an analytical expression for the velocity, v_z, as a function of position, x, can be easily derived:

$$v_z = \frac{\rho g \delta^2}{2\eta}\left[1 - \left(\frac{x}{\delta}\right)^2\right] \tag{18}$$

In Figure 6, we show the velocity profile for the Newtonian and the Bingham fluids. This plot is obtained by using the *Mathematica*® commands:

```
sol1 = myODEsoln[bc]
plt1 = Plot[vz[x] /. sol1, {x, 0, δ}, PlotStyle → RGBColor[0, 0, 1]]
```

A comparison of the velocity profile obtained using the analytical solution for the Newtonian fluid and the velocity profile corresponding to the Bingham fluid shows that the latter is flat near the surface of the liquid film. In fact, we have a non-zero velocity gradient only when $\tau_{xz} > \tau_0$. This behavior is typical of Bingham fluids.

VI- Expressions of volumetric flow rates

Problem statement. Derive expressions of volumetric flow rates for pipe flow of Bingham and power-law fluids using symbolic computations with *Mathematica*®.

Solution.

1- Power-law fluid case

First, we find the expression of the shear stress, τ_{rz}, as a function of the radial position, r:

```
sol3 = DSolve[D[r τrz[r], {r, 1}] == -ΔP / L r, τrz[r], r]
τrz[r] = sol1[[1, 1, 2]] /. C[1] → 0
```

We get the following result:

$$\tau_{rz} = -\frac{\Delta P\, r}{2L} \tag{19}$$

Then, we determine the velocity distribution using the symbolic command, *Dsolve*,

```
sol4 = DSolve[D[vz[r], {r, 1}] == -(-τrz[r] / κ)^(1 / n), vz[r], r]
```

$$v_z[r] = \text{sol4}[[1, 1, 2]] \;/.\; C[1] \to \frac{2^{-1/n}\, n\, R \left(\frac{\Delta P\, R}{\kappa\, L}\right)^{\frac{1}{n}}}{1 + n}$$

Finally, the symbolic command, *Integrate*, is used,

```
Q = Integrate[2 Pi r vz[r], {r, 0, R}]
```

and we get the following expression for the volumetric flow rate,

$$Q = \frac{2^{-1/n} \pi R^3 n \left(\frac{R \Delta P}{\kappa L} \right)^{1/n}}{1+3n} \tag{20}$$

2- Bingham fluid case

Just like the treatment above, we start by finding the expression of the shear stress, τ_{rz}, as a function of the radial position, r:

```
sol1 = DSolve[D[r τrz[r], {r, 1}] == -ΔP / L r, τrz[r], r]
τrz[r] = sol1[[1, 1, 2]] /. C[1] → 0
```

We get the following result:

$$\tau_{rz} = -\frac{\Delta P\, r}{2L} \tag{19}$$

In the first part of the derivation, we determine the velocity distribution between $r = (2\tau_0 L)/\Delta P$ and $r = R$ using boundary condition $v_z(R) = 0$ and the symbolic command, *Dsolve*:

```
sol2 = DSolve[D[vz[r], {r, 1}] == (τrz[r] + τ0) / η, vz[r], r]
vz[r] = sol2[[1, 1, 2]] /. C[1] → ΔP R^2/(4 η L) - R τ0/η
```

The symbolic command, *Integrate*, is used to obtain the expression of the volumetric flow rate between $r = (2\tau_0 L)/\Delta P$ and $r = R$,

```
Q1 = Integrate[2 Pi r vz[r], {r, -2 τ0 L / ΔP, R}]
```

In the second part of the derivation, we determine the constant velocity, v_0, between $r = 0$ and $r = (2\tau_0 L)/\Delta P$ using the following symbolic command:

```
v0 = 1 / μ PG (r^2 - R^2) / 4 + τ0 / μ (r - R) /. r → 2 τ0 L / ΔP
```

This is nothing more than expressing the continuity of the velocity at $r = (2\tau_0 L)/\Delta P$. In fact, we have written that $v_0 = v_z((2\tau_0 L)/\Delta P)$ in the above *Mathematica*® statement.

The symbolic command, *Integrate*, is used to obtain the expression of the volumetric flow rate between $r = 0$ and $r = (2\tau_0 L)/\Delta P$,

```
Q2 = Integrate[2 Pi r v0, {r, 0, 2 τ0 L / ΔP}]
```

and we get the following expression for the overall volumetric flow rate,

$$Q = \frac{\pi R^4 \Delta P}{8\eta L} - \frac{\pi R^3 \tau_0}{3\eta} + \frac{2\pi \tau_0^4 L^3}{3\eta \Delta P^3} \tag{21}$$

V- Non-Newtonian fluid model determination

Problem statement. Wilkes[5] provides representative values of the volumetric flow rate versus the applied pressure gradient for horizontal flow in a pipe. These values are reproduced in Table 1. The pipe radius is equal to $R = 0.01\,\mathrm{m}$. Use these representative values, in conjunction with the analytical expression of the volumetric flow rates determined in the previous section, to compute the parameters of the constitutive equation.

Solution. First, we compute the following sum:

$$J = \sum_{i=1}^{10} \left(Q_i^{rep} - Q_i^{th} \right)^2 \tag{22}$$

where Q_i^{rep} and Q_i^{th} are the representative value and analytical expression of the volumetric flow rate. Then, we use the built-in command of *Mathematica*®, *FindMinimum*, to determine the values of n and κ for the power-law model and τ_0 and η for the Bingham model that minimize the objective function J. The approach use here is the least squares method. For the power-law model, we find $\mathrm{n} = 0.437$ and $\mathrm{k} = 6.708$ while for the Bingham model the result is $\tau_0 = 77.55$ and $\eta = 0.0326$. The value of the sum given by equation (22) is 9.89×10^{-6} for the Bingham model and 2.67×10^{-7} for the power-law model. Thus, we conclude that the power-law model fits the representative data better.

Conclusions

We presented the solution of four non-Newtonian fluid mechanics problems using *Mathematica*®. The velocity profile is obtained for the horizontal flow of power-law fluids in pipes and annuli and for the vertical laminar flow of a Bingham fluid. These problems have split boundary conditions and we applied the shooting techniques to solve them. Analytical expressions of volumetric flow rates for pipe flow of the Bingham and power-law fluids were derived using *Mathematica*®. The parameters of the constitutive equation of non-Newtonian fluids were obtained from representative data of flow rates measured under different applied pressure gradients in a horizontal pipe. These problems are simple enough to constitute an excellent introduction to the field of non-Newtonian fluid mechanics. Students at the National Institute of Applied Sciences in Tunis perform well despite no previous knowledge of *Mathematica*®.

References

[1] http://library.wolfram.com/infocenter/search/?search_results=1;search_person_id=1536 .

[2] Wolfram, S., *Mathematica® , A System for doing Mathematics by Computer*, Addison-Wesley, Redwood City, 1988.

[3] http://www.polymath-software.com

[4] Cutlip, M. B. and M. Shacham, *Problem Solving in Chemical Engineering with Numerical Methods*, Prentice Hall, Upper Saddle River, 1999.

[5] Wilkes, J. O., *Fluid Mechanics for Chemical Engineers*, Prentice Hall, Upper Saddle River, 1999.

Nomenclature

g : gravitational acceleration ($\mathrm{m/s^2}$)

Q : volumetric flow rate ($\mathrm{m^3/s}$)

L : pipe length (m)

n : power-law exponent

ΔP : pressure difference (Pa)

R : pipe radius (m)

R_1 , R_2 : annulus radiuses (m)

r : radial position (m)

v_z : velocity (m/s)

z : axial position (m)

κ : power-law consistency index ($\mathrm{N.s^n/m^2}$)

δ : film thickness (m)

λ : relaxation parameter (s)

η : viscosity ($\mathrm{kg/m.s^2}$)

η_0 : zero-shear viscosity ($\mathrm{kg/m.s^2}$)

η_∞ : infinite-shear viscosity ($\mathrm{kg/m.s^2}$)

ρ : density ($\mathrm{kg/m^3}$)

τ_0 : yield stress (kg/m.s)

τ_{rz} : shear stress (kg/m.s)

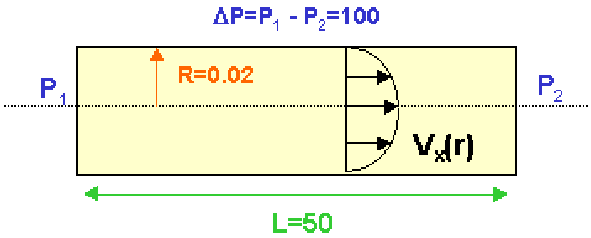

Figure 1 - Flow of Carreau and power-law fluids in a pipe

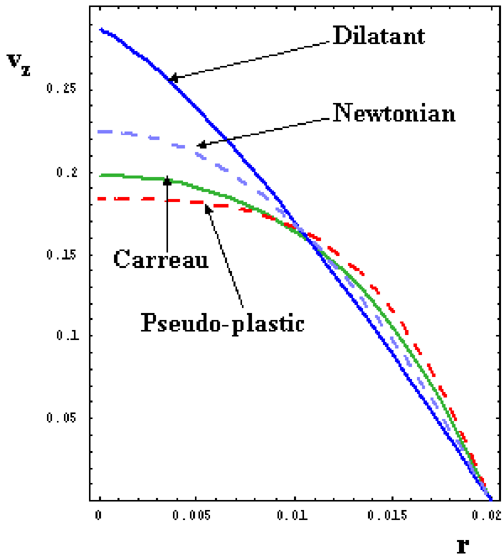

Figure 2 - Velocity profiles of dilatant, pseudo-plastic, Carreau and Newtonian fluids in a pipe

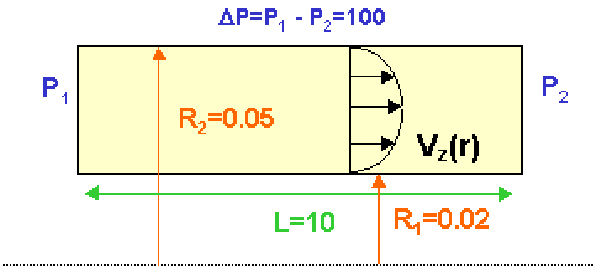

Figure 3 - Flow of Carreau and power-law fluids in an annulus

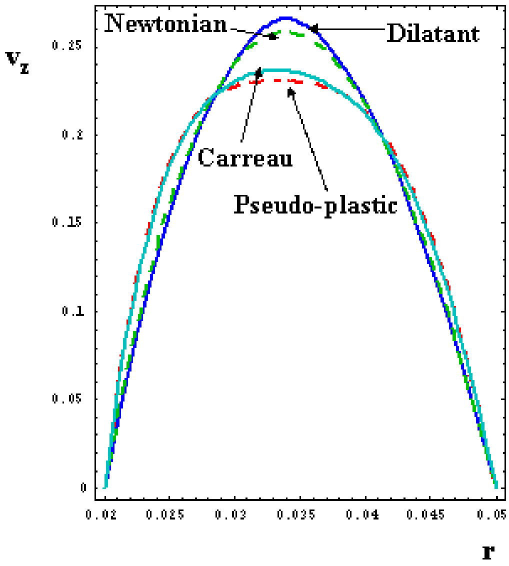

Figure 4 - Velocity profiles of dilatant, pseudo-plastic, Carreau and Newtonian fluids in an annulus

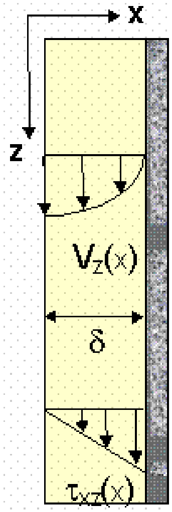

Figure 5 - Vertical flow of a Bingham fluid in a liquid film

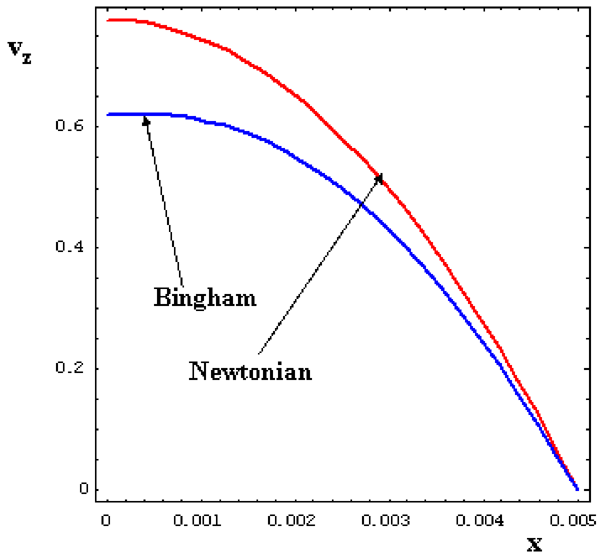

Figure 6 - Velocity profiles of Bingham and Newtonian fluids in liquid film

$\Delta P/L \quad (Pa/m)$	$10^5 \times Q \quad (m^3/s)$
10000	5.37
20000	26.4
30000	68.9
40000	129
50000	235
60000	336
70000	487
80000	713
90000	912
100000	1100

Table 1 - Volumetric flow rate versus pressure gradient