What is rheology anyway?

Rheology = the study of deformation and flow.

To the layperson, rheology is:

• Mayonnaise does not flow even under stress for a long time; honey always flows.
• Silly Putty bounces (is elastic) but also flows (is viscous).
• Dilute flour-water solutions are easy to work with but doughs can be quite temperamental.
• Corn starch and water can display strange behavior — poke it slowly and it deforms easily around your finger; punch it rapidly and your fist bounces off of the surface.

What is rheology anyway?

To the scientist, engineer, or technician, rheology is:

• Yield stresses
• Viscoplastic effects
• Memory effects
• Shear thickening and shear thinning

For both the layperson and the technical person, rheology is a set of problems or observations related to how the stress in a material or force applied to a material is related to deformation (change of shape) of the material.

What is rheology anyway?

Rheology affects:

• Processing (design, costs, production rates)
• End use (food texture, product pour, motor-oil function)
• Product quality (surface distortions, anisotropy, strength, structure development)

Goal of the scientist, engineer, or technician:

• Understand the kinds of flow and deformation effects exhibited by complex systems.
• Apply qualitative rheological knowledge to diagnostic, design, or optimization problems.
• In diagnostic, design, or optimization problems, use or devise quantitative analytical tools that correctly capture rheological effects.
By learning which quantitative models apply in what circumstances.

How?

• Understand the kinds of flow and deformation effects exhibited by complex systems.
• Apply qualitative rheological knowledge to diagnostic, design, or optimization problems.
• In diagnostic, design, or optimization problems, use or devise quantitative analytical tools that correctly capture rheological effects.

Learning Rheology (bibliography)

Descriptive Rheology
Barnes, H., J. Hatton, and K. Walters, An Introduction to Rheology (Elsevier, 1999)

Quantitative Rheology
Morrison, Faith, Understanding Rheology (Oxford, 2001)

Industrial Rheology
Dillon, John and Kurt Wissbrun, Melt Rheology and Its Role in Plastics Processing (Van Nostrand Reinhold, 1990)

Polymer Behavior
Ferry, John, Viscoelastic Properties of Polymers (Wiley, 1980)

Suspension Behavior
Macosko, Chris, Rheology: Principles, Measurements, and Applications (VCH Publishers, 1994)

The Physics Behind Rheology:

1. Conservation laws
   - mass
   - momentum
   - energy

2. Mathematics
   - differential equations
   - vectors
   - tensors

3. Constitutive law = law that relates stress to deformation for a particular fluid

Newtonian fluids: (fluid mechanics)

\[ \tau_{ij} = -\mu \frac{d\gamma_{ij}}{dx} \]

Newton’s Law of Viscosity
This is an empirical law (measured or observed)
May be derived theoretically for some systems

Non-Newtonian fluids: (rheology)

Need a new law or new laws
These laws will also either be empirical or will be derived theoretically

Non-Newtonian Fluid Mechanics

Newtonian fluids:
( shear flow only )

\[ \tau_{ij} = -\mu \frac{d\gamma_{ij}}{dx} \]

Constitutive Equation

Non-Newtonian fluids:
(all flows)

\[ \tau = f [\gamma] \text{ stress tensor} \]

Rate-of-deformation tensor

Stress is a non-linear function (in time and position)

Introduction to Non-Newtonian Behavior

Rheological Behavior of Fluids, National Committee on Fluid Mechanics Films, 1964

<table>
<thead>
<tr>
<th>Type of fluid</th>
<th>Momentum balance</th>
<th>Stress – Deformation relationship (constitutive equation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Newtonian (finite, constant viscosity, ( \mu ))</td>
<td>Navier-Stokes (Cauchy momentum equation with Newtonian constitutive equation)</td>
<td>Stress is a function of the instantaneous velocity gradient</td>
</tr>
<tr>
<td>Newtonian (finite, constant viscosity, ( \mu ))</td>
<td>Newton-Stokes (Cauchy momentum equation with Newtonian constitutive equation)</td>
<td>Stress is isotropic</td>
</tr>
<tr>
<td>Non-Newtonian (finite, variable viscosity ( \eta ) plus memory effects)</td>
<td>Cauchy momentum equation with memory constitutive equation</td>
<td>Stress is a nonlinear function of the history of the velocity gradient</td>
</tr>
</tbody>
</table>

Velocity gradient tensor \( \nabla \)

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Rheological Behavior of Fluids - Newtonian

1. Strain response to imposed shear stress
   • shear rate is constant

2. Pressure-driven flow in a tube (Poiseuille flow)
   • viscosity is constant

3. Stress tensor in shear flow
   • only two components are nonzero

Rheological Behavior of Fluids – non-Newtonian

1. Strain response to imposed shear stress
   • shear rate is variable

2. Pressure-driven flow in a tube (Poiseuille flow)
   • viscosity is variable

3. Stress tensor in shear flow
   • all 9 components are nonzero

Examples from the film of . . . .

Dependence on the history of the deformation gradient
- Polymer fluid pours, but springs back
- Elastic ball bounces, but flows if given enough time
- Steel ball dropped in polymer solution "bounces" (as it does for Newtonian fluids); sometimes more than doubles, sometimes less
- Normal stresses in shear flow
- Die swell

Show NCFM Film on Rheological Behavior of Fluids

Chapter 2: Mathematics Review

Chapter 3: Newtonian Fluid Mechanics

Please review Chapter 2 and Chapter 3
How can we do actual calculations with vectors?

Rule: any vector may be expressed as the linear combination of three, non-zero, non-coplanar basis vectors

\[ \mathbf{a} = a_1 \mathbf{\hat{e}}_1 + a_2 \mathbf{\hat{e}}_2 + a_3 \mathbf{\hat{e}}_3 = \left( \begin{array}{c} a_1 \\ a_2 \\ a_3 \end{array} \right) \]

any vector

\[ \mathbf{a} = a_1 \mathbf{\hat{e}}_1 + a_2 \mathbf{\hat{e}}_2 + a_3 \mathbf{\hat{e}}_3 = \sum_{j=1}^{3} a_j \mathbf{\hat{e}}_j \]

coefficient of \( a \) in the \( \mathbf{\hat{e}}_i \) direction

Einstein Notation

a system of notation for vectors and tensors that allows for the calculation of results in Cartesian coordinate systems.

\[ \mathbf{a} = a_1 \mathbf{\hat{e}}_1 + a_2 \mathbf{\hat{e}}_2 + a_3 \mathbf{\hat{e}}_3 = \sum_{j=1}^{3} a_j \mathbf{\hat{e}}_j = a_j \mathbf{\hat{e}}_j = a_j \mathbf{\hat{e}}_j = a_j \mathbf{\hat{e}}_j \]

Einstein Notation (cont’d)

To carry out a dot product of two arbitrary vectors . . .

\[ \mathbf{a} \cdot \mathbf{b} = (a_1 \mathbf{\hat{e}}_1 + a_2 \mathbf{\hat{e}}_2 + a_3 \mathbf{\hat{e}}_3) \cdot (b_1 \mathbf{\hat{e}}_1 + b_2 \mathbf{\hat{e}}_2 + b_3 \mathbf{\hat{e}}_3) = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_\beta j \cdot j_m \]

Detailed Notation

\[ \mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_\beta j \cdot j_m \]

Einstein Notation

\[ \mathbf{a} \cdot \mathbf{b} = \sum_{j=1}^{3} a_j b_j = \sum_{j=1}^{3} a_\beta j \cdot j_m = a_\beta j \]

Laws of Algebra for Indeterminate Product of Vectors:

NO commutative \( \mathbf{a} \mathbf{b} \neq \mathbf{b} \mathbf{a} \)

yes associative \( \mathbf{a} (\mathbf{b} \mathbf{c}) = (\mathbf{a} \mathbf{b}) \mathbf{c} = \mathbf{a} \mathbf{b} \mathbf{c} \)

yes distributive \( \mathbf{a} (\mathbf{b} + \mathbf{c}) = \mathbf{a} \mathbf{b} + \mathbf{a} \mathbf{c} \)

Tensor – the indeterminate vector product of two (or more) vectors

e.g.: stress \( \mathbf{\sigma} \) velocity gradient \( \mathbf{\nabla} \)

— tensors may be constant or may be variable.

Definitions

dyad or dyadic product – a tensor written explicitly as the indeterminate vector product of two vectors

\[ \mathbf{a} \mathbf{b} \]

\[ \mathbf{a} \]

general representation of a tensor
Mathematics Review

How can we represent tensors with respect to a chosen coordinate system? Just follow the rules of tensor algebra:

\[
\mathbf{m} = (a_{ij} \mathbf{e}_i \mathbf{e}_j + a_{ij} \mathbf{e}_j \mathbf{e}_i)
\]

\[
= a_{ij} \mathbf{e}_i \mathbf{e}_j + a_{ij} \mathbf{e}_j \mathbf{e}_i + a_{ij} \mathbf{e}_i \mathbf{e}_j +
\]

\[
= a_{ij} \mathbf{e}_i \mathbf{e}_j + a_{ij} \mathbf{e}_j \mathbf{e}_i + a_{ij} \mathbf{e}_i \mathbf{e}_j +
\]

\[
= \sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij} \mathbf{e}_i \mathbf{e}_j
\]

Any tensor may be written as the sum of 9 dyadic products of basis vectors.

Summary of Einstein Notation

1. Express vectors, tensors, (later, vector operators) in a Cartesian coordinate system as the sums of coefficients multiplying basis vectors - each separate summation has a different index.
2. Drop the summation signs.
3. Dot products between basis vectors result in the Kronecker delta function because the Cartesian system is orthonormal.

Note:

- In Einstein notation, the presence of repeated indices implies a missing summation sign.
- The choice of initial index (i, m, p, etc.) is arbitrary - it merely indicates which indices change together.

Tensor Invariants

\[
I_2 = \text{trace} \mathbf{A} = \sum_{i=1}^{3} A_{ii}
\]

For the tensor written in Cartesian coordinates:

\[
I_2 = A_{11} + A_{22} + A_{33}
\]

\[
I_4 = \text{trace} (\mathbf{A} \cdot \mathbf{A}) = \mathbf{A} : \mathbf{A} = A_{ij}A_{ji}
\]

\[
I_6 = \text{trace} (\mathbf{A} \cdot \mathbf{A} \cdot \mathbf{A}) = A_{ij}A_{jk}A_{ki}
\]

Note: the definitions of invariants written in terms of coefficients are only valid when the tensor is written in Cartesian coordinates.

4. Differential Operations with Vectors, Tensors

To carry out the differentiation with respect to 3D spatial variation, use the del (nabla) operator.

\[
\nabla = \frac{\partial}{\partial x_1} \mathbf{e}_1 + \frac{\partial}{\partial x_2} \mathbf{e}_2 + \frac{\partial}{\partial x_3} \mathbf{e}_3
\]

We can construct a wide variety of quantities such as: \( \nabla \cdot \mathbf{A} \), \( \nabla \times \mathbf{A} \), \( \nabla (ap) \), etc.

5. Curvilinear Coordinates

These coordinate systems are orthonormal, but they are not constant (they vary with position). This causes some non-intuitive effects when derivatives are taken.

Curvilinear Coordinates (summary)

- The basis vectors are orthonormal.
- The basis vectors are non-constant (vary with position).
- These systems are convenient when the flow system mimics the coordinate surfaces in curvilinear coordinate systems.
- We cannot use Einstein notation on curvilinear coordinates - must use Tables in Appendix C2 (pp464-468).
Chapter 3: Newtonian Fluid Mechanics

Please review this topic.

The solution of Non-Newtonian flow problems will follow the same process as the solution of Newtonian flow problems.

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Mass Balance

Continuity equation: microscopic mass balance
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Momentum Balance

Momentum is conserved.

\[ \begin{align*}
\text{(rate of increase of momentum in } V) & \quad \text{(net flux of momentum into } V) \\
\text{resembles the rate term in the mass balance} & \quad \text{resembles the flux term in the mass balance} \\
\text{Forces} & \text{body (gravity) molecular forces}
\end{align*} \]

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Molecular Forces – this is the tough one

We need an expression for the state of stress at an arbitrary point P in a flow.

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Molecular Forces – this is the tough one (continued)

Think back to the molecular picture from chemistry:

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Molecular Forces – this is the tough one (continued)

The specifics of these forces, connections, and interactions must be captured by the molecular forces term that we seek.

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Molecular Forces – this is the tough one (continued)

• We will concentrate on expressing the molecular forces mathematically;
• We leave to later the task of relating the resulting mathematical expression to experimental observations.

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Chapter 3: Newtonian Fluid Mechanics

Polymer Rheology

Molecular Forces – this is the tough one (continued)

First, choose a surface:
• arbitrary shape
• small

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Consider the forces on three mutually perpendicular surfaces through point $P$.

\[ \vec{a} \] is stress on a "1" surface at $P$
\[ \vec{b} \] is stress on a "2" surface at $P$
\[ \vec{c} \] is stress on a "3" surface at $P$

We can write these vectors in a Cartesian coordinate system:

\[ \vec{a} = a_1 \hat{e}_1 + a_2 \hat{e}_2 + a_3 \hat{e}_3 \]
\[ \vec{b} = b_1 \hat{e}_1 + b_2 \hat{e}_2 + b_3 \hat{e}_3 \]
\[ \vec{c} = c_1 \hat{e}_1 + c_2 \hat{e}_2 + c_3 \hat{e}_3 \]

So far, this is nomenclature; next we relate these expressions to force on an arbitrary surface.

Molecular Forces (continued)

How can we write $f$ (the force on an arbitrary surface $dS$) in terms of the $\Pi_k$?

\[ f = f_1 + f_2 + f_3 \]

$f_1$ is force on $dS$ in 1-direction
$f_2$ is force on $dS$ in 2-direction
$f_3$ is force on $dS$ in 3-direction

There are three $\Pi_k$ that relate to forces in the 1-direction: $\Pi_{11}, \Pi_{12}, \Pi_{13}$

Molecular Forces (continued)

How can we write $f$ (the force on an arbitrary surface $dS$) in terms of the quantities $\Pi_k$?

\[ f = f_1 + f_2 + f_3 \]

$f_1$, the force on $dS$ in 1-direction, can be broken into three parts associated with the three stress components:

First part:
\[ \Pi_{11} \]

Second part:
\[ \Pi_{12} \]

Third part:
\[ \Pi_{13} \]

The sum of these three = $f_1$
f, the force in the 1-direction on an arbitrary surface dS is composed of THREE parts.

\[ f = \Pi_1 \cdot \hat{e}_1 \cdot dS + \Pi_2 \cdot \hat{e}_2 \cdot dS + \Pi_3 \cdot \hat{e}_3 \cdot dS \]

Using the distributive law:

\[ f = \hat{n} \cdot (\Pi_1 \hat{e}_1 + \Pi_2 \hat{e}_2 + \Pi_3 \hat{e}_3) \cdot dS \]

Total stress tensor (molecular stresses)

Assembling the force vector:

\[ f = f_1 \hat{e}_1 + f_2 \hat{e}_2 + f_3 \hat{e}_3 \]

\[ = dS \hat{n} \cdot (\Pi_1 \hat{e}_1 + \Pi_2 \hat{e}_2 + \Pi_3 \hat{e}_3) \hat{e}_1 \]
\[ + dS \hat{n} \cdot (\Pi_1 \hat{e}_1 + \Pi_2 \hat{e}_2 + \Pi_3 \hat{e}_3) \hat{e}_2 \]
\[ + dS \hat{n} \cdot (\Pi_1 \hat{e}_1 + \Pi_2 \hat{e}_2 + \Pi_3 \hat{e}_3) \hat{e}_3 \]

\[ = dS \hat{n} \cdot \left[ \Pi_1 \hat{e}_1^1 + \Pi_2 \hat{e}_2^2 + \Pi_3 \hat{e}_3^3 \right] \]

linear combination of dyadic products = tensor

The same logic applies in the 2-direction and the 3-direction.

\[ f = dS \hat{n} \cdot \left[ \Pi_1 \hat{e}_1^1 + \Pi_2 \hat{e}_2^2 + \Pi_3 \hat{e}_3^3 \right] \]

Assembling the force vector:

\[ \left[ \begin{array}{c}
\frac{\partial}{\partial t} \rho \mathbf{v} dV + \int \rho dV + \int \mathbf{f} dV + \int \mathbf{f} dS
\end{array} \right] = 0 \]

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Momentum Balance (continued)

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}) dV - \int \nabla \cdot (\rho \mathbf{v}) dV + \int \rho \mathbf{g} dV + \int \mathbf{F} dV = 0
\]

Our choice:

- positive compression (pressure is positive)

Gauss Divergence Theorem

Final Assembly:

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}) dV = -\int \nabla \cdot (\rho \mathbf{v}) dV + \int \rho \mathbf{g} dV - \int \nabla \cdot \mathbf{F} dV
\]

Because \(V\) is arbitrary, we may conclude:

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \rho \mathbf{g} + \nabla \cdot \mathbf{F} = 0
\]

Microscopic momentum balance

After some rearrangement:

\[
\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla \cdot \mathbf{F} + \rho \mathbf{g}
\]

Equation of Motion

Now, what to do with \(\mathbf{F}\)?