MODELING AND SIMULATION OF NON-NEWTONIAN FLUID FLOW USING COMSOL MULTIPHYSICS®

Galina Shugai

COMSOL AB, 111 40 Stockholm, Sweden

ABSTRACT

This paper presents an overview of the capabilities of COMSOL Multiphysics® for simulating non-Newtonian fluids, with an emphasis on multiphysics. It outlines the COMSOL implementation of inelastic and viscoelastic non-Newtonian fluid models and reviews the software's ability to couple fluid flow with heat transfer, structural deformation, and multiphase flow modeling.

FLUID FLOW MODELING

COMSOL Multiphysics is a finite element-based simulation software designed for modeling and solving physical problems involving processes such as fluid flow, heat transfer, and structural deformation. Starting from individual physics, it is possible to combine multiple physical phenomena in the COMSOL environment to simulate real-world behavior. COMSOL includes several interfaces specifically tailored for simulating flows with complex rheological behavior.

Fluid motion can be described using simplified mathematical models or engineering correlations for specific cases. However, the most comprehensive description is based on fundamental conservation laws: the continuity equation for mass conservation and the Navier–Stokes equations for momentum conservation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \tau + \mathbf{f}, \tag{2}$$

where $\mathbf{u}$ is the velocity field, p is the pressure, ρ is the fluid density, τ is the stress tensor, and $\mathbf{f}$ is the body force (e.g., gravity).

Inelastic non-Newtonian models

Solving momentum conservation equations requires specifying the rheological behavior of the fluid through the stress tensor τ, which must be defined by a suitable constitutive equation. For an incompressible Newtonian fluid, the stress tensor can be written as

$$\tau = 2\mu\mathbf{D},\ \mathbf{D} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^\top\right) \tag{3}$$

where μ is the viscosity.

However, many fluids deviate from this simple relationship. COMSOL provides a comprehensive suite of built-in constitutive models for both inelastic and viscoelastic behaviors. Inelastic non-Newtonian models typically follow the form of Eq. 3, but with viscosity replaced by an apparent viscosity, often calculated from the shear rate $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$. These models fall into two broad categories: those with yield stress behavior (viscoplastic) and those without. For fluids without yield stress behavior, COMSOL includes models such as the Power Law:

$$\mu = m(\max(\dot{\gamma}, \dot{\gamma}_{\text{min}}))^{n-1} \tag{4}$$

where m and n are scalars. For $n > 1$, the fluid is shear thickening (dilatant); for $n < 1$, shear thinning (pseudoplastic); and $n = 1$ corresponds to a Newtonian fluid. The lower bound for the share rate $\dot{\gamma}_{\text{min}}$ is introduced to avoid infinite viscosity at zero shear rate when $n < 1$.

The Ellis and Sisko models offer enhanced accuracy in different regimes. The Ellis model is a three-parameter model that is usually better than the power-law in matching experimental measurements in low and medium shear-rate regimes. The Sisko model includes both the power law region and an infinite shear plateau.

The Carreau–Yasuda model can be described by the equation

$$\mu = \mu_\infty + (\mu_0 - \mu_\infty)\left[1 + (\lambda\dot{\gamma})^a\right]^{\frac{n-1}{a}} \tag{5}$$

where λ is the time constant, μ_0 is the zero-shear viscosity, μ_∞ is the infinite-shear viscosity, and a is the transition parameter. Eq. 5 allows the recovery of the Carreau, Cross, and Cross-Williamson models through specific parameter choices.

Viscoplastic fluid behavior is characterized by the existence of a yield stress, denoted as τ_y, a threshold that must be exceeded before significant deformation occurs. Constitutive models for such fluids include this yield stress, which introduces numerical challenges due to the inherent discontinuity. To address these challenges, the Papanastasiou regularization method[2] is employed in COMSOL, thus enabling the modeling of both yielded and unyielded regions in a continuous manner. Five models for fluids exhibiting yield stress behavior are available: Bingham, Herschel–Bulkley, Casson, DeKee–Turcotte, and Robertson–Stiff. For example, the Bingham plastic model with Papanastasiou regularization is expressed as:

$$\tau = \tau_y\left(1 - e^{-m\dot{\gamma}}\right) + \mu_p\dot{\gamma} \tag{6}$$

where μ_p is the plastic viscosity, and m is a regularization parameter that controls the sharpness of the transition between unyielded and yielded behavior.

COMSOL also offers the Houska model, a viscoplastic constitutive model. It extends the Bingham plastic model by incorporating a shear-rate-dependent viscosity, allowing it to better represent complex flow characteristics of structured fluids such as suspensions and pastes. The model is particularly useful in capturing thixotropic behavior and structural recovery in time-dependent non-Newtonian fluids.

The predefined models can be extended or customized using the equation-based modeling tools to implement user-defined constitutive relations, time-dependent viscosity functions, or microstructural evolution equations relevant to thixotropic and viscoplastic materials.

In COMSOL, it is possible to model the flow of non-Newtonian fluids through porous media using the concept of an apparent shear rate. This quantity represents the equivalent shear rate that would produce the same pressure drop in a porous medium as in a free-flow scenario for a given non-Newtonian fluid. The apparent shear rate is expressed as:

$$\dot{\gamma}\text{app} = \alpha \frac{|\mathbf{u}|}{\sqrt{\kappa \varepsilon_{\mathrm{p}}}} \tag{7}$$

where α is a correction factor that depends on the porous structure, κ is the permeability, and ε_{p} is the porosity of the medium. The value of α is not universal; it must be determined experimentally or estimated using pore-scale simulations.

Viscoelastic models

To model viscoelastic effects, the stress tensor is expressed as the sum of a viscous and an elastic contribution:

$$\tau = 2\mu_{\mathrm{S}}\mathbf{D} + \mathbf{T}_e, \tag{8}$$

where $\mathbf{T}_e$ is the elastic (or viscoelastic) stress tensor which is often represented as a sum of the individual modes: $\mathbf{T}_e = \sum_m \mathbf{T}_{e_m}$. The multimode formulation provides a more accurate description of the rheological behavior of fluids with a spectrum of relaxation times typically resulting from the polydispersity of macromolecules.

To complete the system of equations, a constitutive relation must be specified for each mode. Only differential constitutive models are available in COMSOL. These models can be formulated in different ways, depending on the choice of dependent variables. In a stress formulation, the extra stress tensor is the primary dependent variable. Alternatively, in a conformation formulation, an intermediate structural variable—the conformation tensor $\mathbf{C}$—is used, with the stress determined as an explicit function of $\mathbf{C}$.

Several commonly used constitutive models can be expressed as hyperbolic partial differential transport equations in the stress formulation[1]:

$$\mathcal{U}(\mathbf{T}_e) + \mathbf{f}_{\mathrm{r}}(\mathbf{T}_e) = \frac{\mu_e}{\lambda_e}\mathbf{f}_{\mathrm{p}}(\mathbf{T}_e) \tag{9}$$

Here, $\mathbf{f}_{\mathrm{r}}$ and $\mathbf{f}_{\mathrm{p}}$ are model-specific functions representing relaxation and viscous effects, respectively, λ_e is the relaxation time, and μ_e denotes the elastic viscosity. The function $\mathcal{U}(\mathbf{T})$ is the upper-convected derivative:

$$\mathcal{U}(\mathbf{T}_e) = \frac{\partial \mathbf{T}_e}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{T}_e - \left(\nabla \mathbf{u} \cdot \mathbf{T}_e + \mathbf{T}_e \cdot \nabla \mathbf{u}^T\right) \tag{10}$$

This derivative is essential in viscoelastic fluid modeling because it ensures objectivity (frame-independence) of the constitutive equations. In other words, the stress response predicted by the model remains consistent under arbitrary rigid body motions of the coordinate system.

The Oldroyd-B model is one of the simplest constitutive models for viscoelastic fluids, representing a suspension of Hookean springs in a Newtonian solvent with $\mathbf{f}_{\mathrm{r}} = \mathbf{T_e}$ and $\mathbf{f}_{\mathrm{p}} = 1$. Building on this foundation, more advanced models have been developed to capture the complex structural behavior of polymeric fluids. These next-generation models incorporate the concept of networks formed by interacting polymer macromolecules, enabling the continuum-based modeling of polymer melts and concentrated solutions. Additionally to the Oldroyd-B model, COMSOL offers the Giesekus model that includes quadratic nonlinearity due to hydrodynamic drag between polymers, the FENE-P and FENE-CR models with finitely extensible nonlinear elastic (FENE) springs to limit chain extensibility. The LPTT and EPTT models account for network elasticity to resist deformation, improving stability in extensional flows, and the finally Rolie-Poly model that is derived based on tube theory, capturing reptation, chain stretching, and convective constraint release.

The Weissenberg number, Wi, is a dimensionless number that characterizes the relative importance of elastic effects in a flowing viscoelastic fluid $Wi = \lambda_e \dot{\gamma}$ where $\dot{\gamma}$ is the characteristic shear rate. A high Weissenberg number indicates that elastic effects dominate over viscous effects in the flow. In this regime, the elastic stresses can grow rapidly, which can lead to convergence issues or unphysical results. This problem is particularly severe in geometries with sharp corners and in flows with strong extensional components. Overcoming high Weissenberg number problems requires careful numerical stabilization and sometimes simplified modeling approaches.

MULTIPHYSICS COUPLINGS INVOLVING NON-NEWTONIAN FLUIDS

One of the major advantages of using COMSOL is its seamless integration of multiphysics: non-Newtonian fluid flow can easily be coupled with other physical processes in the same model. This is particularly important for complex fluids, whose behavior often depend on temperature, chemical composition, or interactions with solid structures.

Non-isothermal flow modeling

Modeling non-isothermal flow is essential in many industrial applications involving non-Newtonian fluids, because of the strong coupling between the flow, stress, and thermal fields, which significantly affect the material response. COMSOL addresses these problem through the Non-Isothermal Flow multiphysics interface, which couples the fluid flow equations with the heat transfer equations. The heat transfer equation is expressed as:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = k \nabla^2 T + Q \tag{11}$$

where ρ is the fluid density, C_p is the specific heat capacity, k is the thermal conductivity, and Q is the internal heat source term. The Nonisothermal Flow interface is pre-configured to include the heat source Q that includes several contributions:

$$Q = 2\mu_{\mathrm{S}} \mathbf{D} : \mathbf{D} + \alpha \, \mathbf{T}_e : \mathbf{D} + (1 - \alpha) \frac{\mathrm{tr}(\mathbf{T}_e)}{2\lambda_e(T)} \tag{12}$$

The first term represents viscous heating, that is present in both Newtonian and non-Newtonian fluids. For viscoelastic flows, the internal heat generation includes an irreversible dissipation term and a reversible component. In COMSOL, the reversible part is neglected ($\alpha = 1$).

Heating generally reduces viscosity due to increased molecular mobility. As temperature rises, polymer chains or molecular segments move more freely, leading to a decrease in flow resistance. This temperature-dependent behavior is modeled in COMSOL Multiphysics using thermal functions:

$$\frac{\mu_s(T)}{\mu_s(T_0)} = \alpha_T(T) \tag{13}$$

For viscoelastic flows, it is assumed that both the relaxation time and elastic viscosity vary with temperature:

$$\frac{\mu_e(T)}{\mu_e(T_0)} = \frac{\lambda_e(T)}{\lambda_e(T_0)} = \alpha_T(T) \tag{14}$$

where $\alpha_T(T)$ is a temperature-dependent scaling function. Several thermal function models are available, including Arrhenius, WLF (Williams–Landel–Ferry), exponential forms, and user-defined functions.

Chemorheology

In many industrial applications involving non-Newtonian fluids—such as thermoset polymers, adhesives, and resins—viscosity is highly dependent on both temperature and the degree of cure. As curing progresses, chemical cross-linking between polymer chains restricts molecular motion, leading to a significant rise in viscosity. In the later stages, the system may undergo gelation, where viscosity increases dramatically.

This rise in viscosity can enhance viscous heating, which in turn raises the local temperature and further accelerates the curing process. The resulting interplay between thermal effects, curing kinetics, and viscous dissipation produces a highly nonlinear and tightly coupled behavior in the viscosity field.

Accurate simulation of such systems requires the simultaneous solution of the flow, heat transfer, and curing. The curing process is typically modeled using temperature-dependent reaction kinetics, where the degree of cure, c, evolves over time. A common form of the cure-kinetics equation is:

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = R(T, c) \tag{15}$$

Available reaction models include the Sestak–Berggren, Kamal–Sourour, and n-th order. To capture the sharp increase in viscosity during the curing of thermosetting polymers—particularly when the polymer network is close to gelation—the Castro–Macosko and percolation-based viscosity models are included.

Curing reactions are typically exothermic, releasing heat as crosslinking progresses:

$$Q_\mathrm{r} = H_r \frac{d\alpha}{dt} \tag{16}$$

where H_r is the total heat of reaction. COMSOL provides a dedicated coupling that automatically incorporates this source term into the heat transfer equation (Eq. 11).

Fluid–Structure Interaction

Fluid–Structure Interaction (FSI) refers to coupling fluid flow with solid mechanics so that a deformable structure and the fluid mutually influence each other. COMSOL supports fully coupled FSI simulations even for non-Newtonian fluids. For example, one could simulate the flow of an inelastic or a viscoelastic fluid flowing through an elastic tube, capturing how the fluid pressure deforms the structure and how that deformation in turn alters the flow.

Multiphase Flow and Free Surfaces

Many non-Newtonian fluid applications—such as coating, mold filling, and extrusion—involve free surfaces or multiphase flows. COMSOL provides several methods for simulating two-phase or multiphase flows with interface tracking, including the Level Set, Phase Field, and Moving Mesh (ALE) approaches. These methods can be directly coupled with non-Newtonian fluid models using predefined two-phase flow multiphysics couplings.

The beads-on-string structure is a phenomenon observed in thinning viscoelastic filaments, surface tension and elastic stresses cause the filament to form droplet-like beads connected by thin threads. It is a classic example that is used to verify numerical simulations. The problem is solved in COMSOL using the Oldroy B model and Moving Mesh (ALE) functionality. **Fig. 1** shows the evolution of the filament at different times. The results are in good agreement with the experimental and simulation results presented in other publications[3].

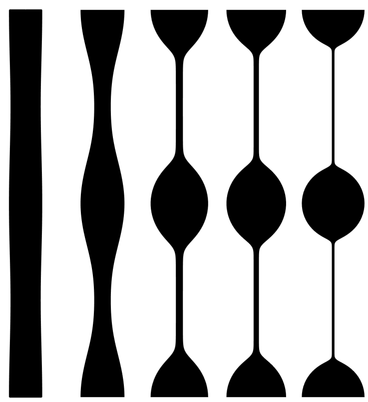

FIGURE 1: Filament profiles at 5 different dimensionless times: 0, 20, 30, 100, and 300

The next example illustrates the filling stage of an injection molding process. Molten polymer is injected into the top of a heated mold initially filled with air. The curing reaction is modeled using the Kamal–Sourour model, while the viscosity's dependence on the degree of cure is described by the Castro–Macosko model. Shear rate dependence is captured using a power-law formulation. **Figure 2** shows the distribution of viscosity and the degree of cure, along with the position of the interface between the air and the polymer melt. The problem is solved using two-phase flow with phase field coupling, non-isothermal flow, and curing reaction heat coupling.

In conclusion, the COMSOL Multiphysics simulation software is a practical tool for modeling coupled problems involving non-Newtonian fluid flow. It supports a range of non-Newtonian constitutive models and allows for the integration of flow with thermal, chemical, and structural effects. Built-in methods for handling free-surface and multiphase flows further extend its applicability. These features make it suitable for simulating processes such as polymer curing, coating, and biomedical flows, where complex rheological behavior and multiphysics interactions are significant.

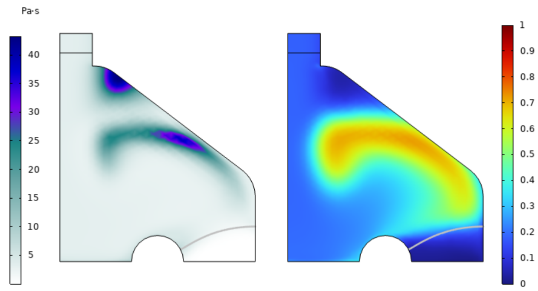

FIGURE 2: Viscosity (left) and degree of cure (right)

REFERENCES

1. Bird R.B., Stewart W.E. and Lighfoot E.N. *Transport Phenomena*, John Wiley, New York, Book Publication, 1960.
2. Papanastasiou T.C Flow of materials with yield *J.Rheol*,**31**, 385–404, 1987.
3. Clasen C., Eggers J., Fontelos M.A, Li J., McKinley G. The beads-on-string structure of viscoelastic threads *J. Fluid Mech.*, **556**, 283–308, 2006.
4. COMSOL Multiphysics, Version 6.3, including the Polymer Flow Module, 2025.