Introduction

Elastic stress has been incorporated into FLOW-3D® to emulate viscoplastic materials, which are materials which behave as solids up to a yield stress, beyond which they behave like a viscous liquid. The state of stress for a Newtonian viscous liquid is

$$T = 2\mu\dot{E}$$  \hspace{1cm} (1)

where $\mu$ is the viscosity coefficient, $\dot{E}$ is the strain-rate tensor, and $T$ is the Cauchy stress tensor. By contrast, the state of stress for a Hookean elastic solid [1] is

$$T = 2GE$$  \hspace{1cm} (2)

where $G$ is the elastic modulus, and $E$ is the strain tensor.

The incremental elastic stress model recently incorporated into FLOW-3D® computes the elastic stress using linear Hookean theory (Equation 2 above). Although this constitutive equation predicts only a linear response to stress, implementation as an incremental model, in which the stress changes in each time step are accumulated, allows the prediction of highly nonlinear responses. This works because the response within each small time step can be well approximated as linear. Pictorially, with this model, FLOW-3D® predicts the total stress as a summation of the viscous stress and the elastic stress, as shown in Figure 1.

![Figure 1: Pictorial view of viscoplastic model, showing the relationship between the elastic and viscous stresses.](image_url)

Thus the model predicts that the total state of stress is a summation of the viscous stress and the elastic stress; one of these dominates, depending on the local strain and strain rate. Suppose a rod of viscoplastic material, as described by this model, undergoes a fixed amount of strain, imposed over a very short time. This model would predict a corresponding rise in elastic stress that is linearly proportional to the strain. Also, during the short time of the strain imposition, the viscous stress would become significant, only to fall to zero the instant the strain imposition ceased. If further strain were to be imposed to a point such that the elastic stress surpasses the yield stress, the material would yield and begin to flow as a viscous liquid with viscosity $\mu$. 
**Elastic stress model**

Because *FLOW-3D®* uses a fixed mesh Eulerian approach to model fluid flow through the domain, this same approach was used to compute the elastic stress. The elastic stress at a point in time, \( t \), for an element of fluid is

\[
\tau_E(\xi, t) = \int_{-\infty}^{t} 2G \dot{\varepsilon}(\xi, t') dt'
\]

where \( \tau_E \) is the elastic stress tensor and \( \xi \) represents a material coordinate (i.e. a small, but finite volume of the material) which translates and rotates with the deforming material. \( \dot{\varepsilon} \) is the local strain rate tensor, computed from

\[
\dot{\varepsilon} = \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]
\]

where \( \mathbf{u} \) is the local velocity vector. Equation 3 is the basis of the incremental stress model. Written for the Eulerian (fixed grid) coordinate system, the time rate of change of Equation 3 is

\[
\left( \frac{\partial \tau_E}{\partial t} \right)_x + \mathbf{u} \cdot \nabla \tau_E = 2G \dot{\varepsilon}(\mathbf{x}, t)
\]

where \( \tau_E \) here is the elastic stress tensor represented in the fixed coordinate system, \( \mathbf{x} \), which corresponds to the mesh used in *FLOW-3D®*.

The current value of stress is a function of the past history of the fluid element. Fluid that enters the domain has a null state of stress, unless specified otherwise at boundaries. Also, the initial condition at the beginning of the simulation has a null state of stress, unless specified otherwise by the initial conditions.

In order to predict yielding effects, the Mises yield condition is used. This condition is

\[
II_{\tau_E} = \frac{Y^2}{3}
\]

where \( II_{\tau_E} \) is the second invariant of the elastic stress tensor \( \tau_E \) and \( Y \) is the yield stress limit, a user-defined parameter. In regions of the material where the elastic stress (measured by \( II_{\tau_E} \)) exceeds the yield criterion, the elastic stress is relaxed such that the condition in Equation 6 is met:

\[
\tau_E^* = \sqrt[3]{\frac{2Y^2}{3II_{\tau_E}}} \tau_E
\]

where \( \tau_E^* \) is the yield-limited elastic stress tensor.

Equation 5 is discretized spatially and temporally and the resulting value of the stress tensor \( \tau_E \) is added to the momentum equation as

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \left\{ \nabla \left[ \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \mathbf{F}_h + \nabla \cdot \tau_E^* \right\}.
\]

The last term in Equation 8 is the divergence of elastic stress.

**Computation of the strain rate tensor, \( \dot{\varepsilon} \)**

The strain rate tensor, \( \dot{\varepsilon} \), is determined from the computed flow velocities. The normal components of \( \dot{\varepsilon} \) are computed at the cell center, while the shear components are calculated at the cell edges [2]. Figure 2 shows a typical computational cell and the stress components. The shear components are computed on the cell edges for computational convenience when computing the divergence of the stress tensor for inclusion into the equation of motion for the fluid.
At free surface interfaces, the external fluid is presumed to be a gas or vapor which exerts negligible stress on the fluid surface. Therefore, $\mathbf{n} \cdot \mathbf{\tau}_E = 0$ at such interfaces. In FLOW-3D®, the principal directions in which free surfaces face and the status of neighboring cells are known. From this information, the appropriate components of $\mathbf{\tau}_E$ are set to zero at free surfaces to ensure that the aforementioned condition is met. At interfaces with solid walls or obstacles, the fluid velocity in the cell neighboring the wall (or obstacle) and the velocity of the wall (or obstacle) are used to compute the strain rate in Equation 4.

**Required parameters for the elastic stress model in FLOW-3D®**

To activate the elastic stress model, the flag `ielast` in the `xput` namelist in the FLOW-3D® input file is set to a positive integer value. For an elastic material, the shear elastic modulus (value $G$ above) must be specified. It is specified as `emod` in the `props` namelist. Also, the yield stress limit is specified as `yield` in the `props` namelist. Specifying yield to be 0 tells the model that the yield stress is infinite; no yielding occurs. All elastic properties act on fluid 1 regions, and the model currently has been designed only for one-fluid models. An excerpt from a sample prepin file is shown below. The required parameters are indicated.

```
$xput
  remark='units are ...',
  twfin=5.0e-5,
  itb=1,
  dtmin=1e-14,
  hpldt=5e-8,
  ihelp=2,
  iorder=3,
  pltldt=5.0e-7,
  delt=1e-9,
  ifvis=0,
  iadiz=1,omega=1.0,
  gz=-981.0,
  sprtdt=5.0e-8,
  ielast=1,
$end

$limits
$end

$props
  rhof=1.0,
  emod=10.0e8,
  yield=0.0e6,
  mu1=0.1,
$end
```

![Figure 2: Computational cell showing locations of components of strain rate tensor](image-url)
**Examples**

**Bouncing ball**
Figure 3 shows the simulation of a bouncing ball. The ball is defined as a sphere, 2cm in radius, with an initial downward velocity of 40 cm/s. The ball strikes the wall boundary, and is deflected at a velocity of about 20 cm/s. The collision is not perfectly elastic because a viscosity is specified for the solidified fluid, and the fluid tends to adhere somewhat to the solid surface during lift-off.

**Flexing beam**
Figure 4 shows the simulation of a beam flexing under the influence of gravity. The beam has a density of 1 g/cm$^3$, shear modulus of 10000 Pa, and infinite yield stress. Its length is 0.75 cm and its thickness is 0.3 cm. This is a two-dimensional simulation.

**Yielding flow**
Figure 5 shows a simulation of a Bingham fluid being forced through a slot by a uniform pressure gradient. The fluid in this case has a shear modulus of 1000 Pa, and a yield stress of 100 Pa. The slot is 0.5 cm wide, and the imposed pressure at the upstream end of the channel is 500 Pa, and it is 0 Pa at the downstream end. The length of the channel is 2 cm.

![Figure 3: Simulation of bouncing ball. Ball is a solidified “fluid” with shear modulus 10000 Pa, density 1 g/cm$^3$. No yield stress or gravity.](image)

![Figure 4: Simulation of flexing beam due to gravity. This is an example of the large deformation capabilities of the model. The beam is a solidified “fluid” with shear modulus 10000 Pa, density 1 g/cm$^3$, thickness 0.3 cm, and length (from the wall surface) 0.75 cm. No yield stress.](image)
Figure 5: Steady-state result of yielding plastic flow. Notice the plug flow region through most of the channel width, with shearing occurring only near the wall boundaries. Fluid has a shear modulus of 1000 Pa, and a yield stress of 100 Pa.

Remarks

A model to accurately predict the elastic response in a transient, three-dimensional fixed-grid CFD modeling package has been implemented. Furthermore, this forms the basis of a number of potential models: thermoelastic stress, viscoelastic materials, and flows containing both solid-like and liquid-like regions. To get there, the model needs to be implemented for the two-fluid model, inclusion of thermal effects is needed, and a relaxation parameter is needed to predict the behavior of viscoelastic materials.

References
