A THREE DIMENSIONAL FINITE ELEMENT MODEL OF BIOFILM
SUBJECTED TO FLUID FLOW AND ITS APPLICATION TO
PREDICTING DETACHMENT POTENTIAL

By

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Peter Norman Gammelgard

July, 2006
To all who have supported me
in my endeavors, academic and otherwise.
Thank you.
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ABSTRACT

Microbial biofouling of wetted surfaces can adversely impact the hydrodynamic performance of pressurized conduits. These impacts are due, in part, to the viscoelastic material properties of biofilm. Of particular interest is the response of biofilm to changing hydrodynamic conditions and its effect on potential for biofilm removal. The goal of this research was two fold; 1) to develop a three dimensional numerical model, incorporating the viscoelastic material description of biofilm, to simulate the response of biofilm to varying hydrodynamic conditions and 2) use this model to identify behavioral characteristics of said biofilm which provide insight into effective removal procedures.

Using a viscoelastic Burger fluid material description for biofilm, a numerical fluid-structure interface model was developed. The model was three-dimensional, allowed various sizes and shapes of biofilm to be defined, and was used in a parametric study to investigate biofilm behavior. The effect of the Burger material parameters and flow velocity were investigated. Additionally, the time scale over which microbial processes may influence biofilm material properties was identified and considered along with the results of the parametric study. Simulations revealed a consistent trend: biofilm clusters in flow channels undergo a transition from decreasing rates of deformation to increasing rates due to the interrelated effects of fluid-induced drag and cluster deformation. The results suggested that biofilm clusters which undergo a transition to accelerated deformation, in a time period shorter than that suggested to be influenced by microbial processes, are destined to eventual detachment. Identification of such behavior has significant impacts on biofilm removal methodology.
INTRODUCTION

Biofilms are ubiquitous on wetted surfaces and are composed of myriad microbes, their byproducts, and the particles which become entrapped in them. While the term “biofilm” is fairly young, ZoBell (1935) is credited as the first to study it. ZoBell’s work primarily focused on the fouling of ship hulls and the detrimental effect on efficiency. As the understanding of the effects of biofilm in an increasingly complex engineering and medical setting improved, interest in investigating biofilm increased, leading to rapid progress which began in the 1970s (Towler, 2004) and continuing through today. Current biofilm research encompasses such fields as biomechanics, medicine, environmental engineering, land rehabilitation, civil engineering and naval science. Although ZoBell penned it in 1935, it is still accurate to say that the “vast economic loss resulting from fouling has instigated extensive investigations of its cause and more particularly of practical methods for its prevention.” The state of the understanding has come a long way in the last 70 years, but the need for further investigation remains strong.

Currently, biofilm research is primarily conducted with one of two aims. Firstly, biofilm can be used to improve the efficiency or efficacy of many processes. For example, sulphate-reducing bacterial biofilms have been shown to reduce hexavalent chromium (Cr(VI)) to insoluble Cr(III) (Smith and Gadd, 2000). This process is significant as Cr(VI) is highly toxic, whereas Cr(III) is insoluble and precipitates out of solution, thereby no longer posing an environmental threat. Additionally, biofilm has been utilized to reduce oxygen penetration in mine waste, in-turn degrading
trichloroethylene, reducing the media permeability, and ultimately reducing the strength of the acid effluent typically associated with such systems (Cunningham, et al., 1997). Secondly, biofilm can cause any number of unwanted results, including contamination and a reduction in system efficiency, typically referred to as biofouling. “This phenomenon can occur in an extremely wide range of situations, from the colonization of medical devices to the production of ultra-pure, drinking and process water and the fouling of ship hulls, pipelines and reservoirs. Although biofouling occurs in such different areas, it has a common cause, which is the biofilm” (Flemming, 2002). In the case of water systems, biofilm frequently leads to contamination problems due to its continuous growth and proclivity to detach, releasing mature microbes, including pathogens, into a water system (Walker et al., 1995). Furthermore, biofilm accumulation has been shown to adversely affect the hydrodynamic efficiency in pipe networks (Zelver, 1979). Considering the frequency of biofilm-covered surfaces, it is quite likely that biofilm is the single most underrepresented hydraulic boundary condition (Towler, 2004). A more complete knowledge of how biofilm interacts with water in a hydraulically dynamic environment may lead to better understanding of methods by which to reduce its ill-effects, as well as provide insight into its potential benefits.

Research Goal

This thesis represents an investigation into the deformation of biofilm when subjected to turbulent fluid flow through a closed conduit utilizing a numerical computer model to simulate, in three dimensions, the behavior of real biofilm subjected to the same
hydrodynamic conditions. An experimentally validated (Towler, 2004) material model was applied in the simulation. The goal of this research was to evaluate the mechanical behavior of biofilm in response to differing hydrodynamic conditions and biofilm properties in three dimensions through the use of the developed numerical model. Specifically, the influence of biofilm material properties and fluid velocity on fluid-induced drag forces and the resulting deformation was considered.
BIOFILM – A BRIEF OVERVIEW

Microbial cells which are free-floating in a fluid are termed planktonic. The word “plankton” is simply a catch-all term to describe “the microscopic animal and plant life found floating in bodies of water” (Neufeldt, 1995). Even treated drinking water can have thousands of living organisms per liter, leading to significant potential for biofilm growth in drinking water systems.

Biofilms form when planktonic cells become ensconced on the fluid boundary, typically a pipe wall or porous media. Once these cells are attached, they grow and reproduce, colonizing the surface. Figure 1, below, shows the general sequence of biofilm formation.

![Biofilm formation: Attachment, Colonization, Growth](image)

Figure 1 - Conceptualization of biofilm formation. Figure shows process of biofilm attachment, colonization, and growth. (CBE, 1995)
Biofilm Structure

Biofilm produces an extracellular polymeric substance (EPS), which helps stabilize and protect the cells it contains, frequently referred to as the matrix. The entire conglomeration of cells, EPS, and even trapped particulates, collectively make up the biofilm.

When observed on the microscale, this matrix is clearly not homogeneous. This heterogeneity is, as Characklis and Marshall (1990) explain, the difference between biofilm and other microbial communities. In addition to its heterogeneity, biofilm is porous with a majority of its volume being water, allowing for significant transport throughout the matrix. As mentioned earlier, particulate matter, such as silt or larger particles such as sand and gravel, can also become entrained within the matrix. In some cases, macroorganisms such as worms may be contained in the biofilm (Characklis and Marshall, 1990).

Biofilm can vary greatly in thickness, geometry and density. Typically, biofilm ranges from 10-1000 μm in thickness. In some cases, thick mats of biofilm can form that exceed 30 mm (Christensen and Characklis, 1990). Some biofilms form uniform-thickness colonies over an entire surface while others are very spotty, covering only portions of a surface (Bakke, 1986). Biofilm geometry and thickness depend greatly on the microbial species diversity as well as growing conditions (Christensen and Characklis, 1990). The mass density of biofilm also varies considerably. Dry mass densities (neglecting the water content) have been recorded as low as 10 kg/m$^3$ (Characklis, 1980) and as high as 105 kg/m$^3$ (Hoehn and Ray, 1973).
As one might suspect, the conditions under which a biofilm grows play a role in its properties. Characklis (1980) showed a correlation between biofilm density and fluid-induced shear stress. In his studies, higher shear stress during growth resulted in higher biofilm density. Additionally, observations made by Trulear (1983) and Bakke (1986) suggest that biofilm thickness is also influenced by bacterial species diversity. Pure cultures of *Psuedomonas aeruginosa*, those cultures containing only *Psuedomonas aeruginosa* microbes, thicknesses rarely exceeded 50 μm while mixed cultures yielded thicknesses in excess of 120 μm (Trulear 1983, Bakke, 1986). Evidence also suggests that density increases with biofilm age (Hoehn and Ray, 1973, Trulear, 1983).

**The Role of the EPS**

Biofilm bacteria commonly produce an extracellular polymeric substance (EPS) matrix (Characklis and Marshall, 1990). This EPS consists primarily of polysaccharides, a carbohydrate compound composed of monosaccharides joined by glycosidic bonds (Towler, 2004). Due to this makeup, biofilm is frequently considered to be a biosynthetic polymer (Flemming et al., 2002.) The physical properties of biofilm are largely dependent on the form of EPS which a specific microbial species produces even though biofilm can entrap particulates from its own growing environment. As such, biofilm is truly an aggregation of microorganisms entrapped in an organic polymer gel (Towler, 2004). Clearly, in understanding the physical behavior of biofilm, a thorough understanding of the EPS and its properties is paramount.
Polymeric chains are formed when monomers are produced and join together. Cross-linking of these chains help strengthen the polymer by resisting rotation and translation with respect to other chains and occurs when adjacent chains are chemically bonded (Rosen, 1993). When hydrated, the biopolymer becomes cross-linked, forming a biopolymer gel. Since as much as 90% of the biofilm organic carbon can take the form of the polymers in the EPS (Bakke, 1986), the EPS is the primary factor in the determination of how biofilm interacts with the substratum as well as its physical properties and interaction with the bulk fluid (Mayer et al., 1999). The bulk fluid in which the biofilm is growing also contributes to the biofilm’s physical properties as it may occupy between 87% and 99% of the biofilm’s volume (Characklis et al. 1981, Zelver 1979). Due to such high volumetric saturation, it seems clear that the bulk solution (typically water) will dictate, in large part, the response of biofilm to hydrostatic stress (Towler, 2004).

**Material Properties**

As mentioned earlier, biofilm is formed when microbes attach themselves to a substratum. The biofilm accumulates and eventually, can detach. This process is typically considered the life cycle of biofilms (Characklis, 1981). EPS is formed during accumulation, and detachment occurs in one of two ways: erosion of individual cells and detachment of larger “chunks” (sloughing) from the biofilm colony. Historically, biofilm has been considered to be a static structure (with the exception of detachment mechanisms). More recently, closer observations of biofilms have revealed many
transient forms in biofilms including streamers (finger-like extrusions), ripples, mushrooms, and dunes (Gjaltema et al., 1994, Stoodley, et al., 1997, Klapper, 2004). In 1999, Stoodley et al. grew mixed-culture biofilms in glass flow cells and observed biofilm structures migrate and elongate under differing flow velocities. This observation demonstrated the dependence of biofilm morphology on local hydrodynamic conditions. This, however, was a study of biofilm kinematics and did not take into account the fluid-induced forces or the biofilm’s mechanical properties. That is to say, while enlightening, the observations were more qualitative than quantitative.

Just as the response of steel or concrete to an applied load is attributed to the intrinsic properties of the steel or concrete, the response of biofilm to induced stresses is due to the intrinsic material properties of that biofilm. Stoodley et al. (1999) conducted simple stress-strain and creep experiments on mixed and pure culture biofilms in situ by observing the structural deformations caused by changes in hydrodynamic shear stress. With those experiments, a simple fluid wall shear stress was taken to be the representative stress acting on the biofilm, thereby greatly simplifying the hydrodynamics of the situation modeled. Of further concern is the fact that the viscoelastic nature of biofilm is discussed and acknowledged yet the viscoelastic nature is forgone in the results by the presentation of a one-dimensional elastic shear modulus. Picioreanu et al. (2001) developed a two-dimensional model of biofilm detachment which includes an elastic response to fluid stress. This multi-dimensional model, while more realistic, still did not agree with the viscoelastic responses observed by other investigators (Ohashi and Harada, 1994, Towler, 2004).
The complex localized flow field surrounding a biofilm cluster must be taken into account to accurately determine the stress response of biofilm to hydrodynamic forces. Furthermore, an appropriate viscoelastic material model must also be employed in any attempt to accurately capture the stress-strain response of biofilm.

**Biofouling**

The term biofouling refers to the undesirable accumulation of microbial biofilm deposits on wetted surfaces (Characklis, 1990). Microbial biofouling occurs in a number of settings. Biofilm can accumulate in water distribution systems, water treatment systems, cooling towers, and other industrial settings (Characklis, 1990). This accumulation can have detrimental effects on the hydraulic performance of such systems. Microbial biofilms also grow on ship hulls, increasing energy loss (ZoBell, 1935). Fouling in the medical field can lead to chronic infection when biofilm grows on medical devices (Costerton et al., 1999). These effects have significant economic impacts. Energy losses due to hydrodynamic drag, replacement of corroded hardware, reduced equipment capacity, and reduced quality all have significant associated costs.

The hydrodynamic impact of biofouling is well documented by observations of increased resistance due to biofilm growth (Bryers and Characklis, 1981). Hydrodynamic resistance is a function of both form drag and surface drag. Surface drag is simply due to the frictional resistance of a fluid boundary. Form drag, on the other hand, and as its name suggests, takes into account the multifaceted forces created as water flows around and interacts with the various forms in the fluid boundary.
Specifically, form drag is an expression of pressure differentials due to boundary layer separation (Cengel and Cimbala, 2006). As biofilm can assume many complex forms (ripples, streamers, mushrooms, etc.), the fluid-induced form drag is potentially significant when considered in addition to the surface drag common to all fluid boundaries. Some have suggested that when the growth of biofilm exceeds the thickness of the laminar sublayer, pressure drop results from increased frictional resistance (McCoy and Costerton, 1982). Both Stoodley et al. (1998) and Towler (2004) suggest that since uniform biofilm accumulation would simply redefine the laminar sublayer, form drag is the operative cause of pressure drop due to biofilm.

If biofilms, with their myriad shapes and forms, are considered as simple, rigid, drag-inducing forms in the flow field, they would contribute to the overall pressure drop observed in many hydraulic systems. There is, however, evidence to suggest that the presence of biofilms is associated with energy loss that is greater than can be accounted for by the size and shape of the biofilm (Picologlou et al. 1980). Picologlou et al. (1980) suggested this was partly due to the viscoelastic material properties of biofilm. Viscoelastic material dissipates energy by its very nature. Viscous flow requires a driving force, and results in deformation. The product of force and displacement is known as work and is expressed in terms of energy. Viscous behavior requires that energy be expended to achieve displacement. In contrast to elastic behavior, however, any expended energy is not stored, and is therefore not conserved.

The results of the Picologlou et al. (1980) study suggest that oscillations in biofilm structures result from fluid flow and energy dissipation cycles. This dissipation
of energy is realized in the increase in overall pressure drop. The role that the
viscoelastic nature of biofilm plays in dissipating energy provides motivation for further
investigation in this area (Hilliard, 2006).
VISCOELASTICITY

Mechanics is the area of study that deals with the behavior of objects subjected to forces. Typically, it is divided into three different fields: the mechanics of rigid bodies (Statics, Dynamics), the mechanics of deformable bodies (Mechanics or Strength of Materials), and mechanics of fluids (Fluid Mechanics) (Beer and Johnston 1988, Gere 2004). In most cases, materials clearly fall into one of these three categories. In some cases, however, material behavior requires a blurring of the lines. Regardless, the goal of the mechanist is to define the relationship between force and deformation.

Forces can fall into two different categories: body forces and surface forces. Body forces are those which act on the entire volume of the body. Electromagnetic and gravitational forces are body forces. Surface forces, as the moniker suggests, refer to those forces which are imparted to a body at its surface. Hydrostatic pressure and friction are examples of surface forces. Any force exerted on a body produces a stress or moment. Stress is a measure of force per unit area. It is further broken into normal and shear stress. Normal stress acts perpendicularly to a surface while shear stress acts tangentially to a surface. Moments are the product of a force and a distance; more specifically, the vector cross-product of the two. A moment, when applied axially to a shaft, can also be called torque.

As mentioned above, the study of deformable solids has been called “strength of materials.” More recently, the discipline has been referred to as “mechanics of materials” as it has come to include not only investigation into the strength of given materials, but also the physical performance of structures and the materials used in them (Gere, 2004).
Deformation, in this context, is defined as the alteration of shape due to applied forces. Deformation is typically reported as either displacement or strain. Displacement is simply the amount of movement a point within a larger body undergoes due to applied forces and is measured with respect to an external coordinate system. Strain, on the other hand, is the local deformation with respect to the body, rather than an external coordinate system. Strain is the elongation (or rotation) per unit length (or angle) and can be divided, like stress, into normal and shear strain. In order to appropriately relate deformation to applied forces, an understanding of material behavior is required.

An elastic material is one which stores energy when it is loaded and releases that energy upon removal of the load. If a material’s strain is directly proportional to the applied stress, that material is considered to be linearly elastic. A fluid is a material which exhibits viscous flow; that is, it deforms continuously when subjected to a shear stress (Cengel and Cimbala, 2006). A linear viscous fluid is one whose strain rate is directly proportional to stress. Water and air are two of the most recognizable fluids. Fluids can be further broken into two categories: compressible and incompressible. Air is compressible; ‘squeezing’ air will reduce its volume. Under standard atmospheric conditions, such as those found in most industrial settings, water behaves as an incompressible fluid. For this reason, water is almost always treated as an incompressible fluid in all applications where extreme conditions are not experienced; squeezing water will result in negligible change in volume. In a general sense, fluids ‘flow’ when not in static equilibrium. A fluid flowing at a constant rate is considered to
be in dynamic equilibrium. Elastic and viscous materials will be discussed in more detail in the following section.

Material Behavior

As mentioned before, a material’s response to applied stress is due to its intrinsic properties. A material’s mechanical behavior is modeled or approximated by a ‘constitutive law’ (Gere, 2006). The development of a material’s constitutive law is a complex process involving investigation into the effects of temperature, strain rate, and magnitude of loading, among other things. (Mase and Mase, 1999). Many investigations have suggested that biofilm is a viscoelastic material (Christensen and Characklis, 1980, Klapper et al. 2002, Stoodley et al. 1999, 2002, Towler et al. 2003, Towler, 2004). Viscoelastic models can be used to represent those varieties of materials exhibiting behaviors which fall between the behavior of deformable, elastic solids and viscous fluids. There is ample evidence to suggest that biofilm does fall in this in-between realm.

As the name implies, viscoelastic models combine characteristics of both viscous and elastic models. Elastic models store mechanical energy while viscous models readily dissipate mechanical energy. Viscoelastic models have the ability to both store and dissipate such energy.

Elasticity

Elastic models respond immediately to applied stress and, once the applied stress is removed, immediately rebound to their original configuration. Linear elastic
models exhibit a linear elastic relationship between stress and strain. “The chief characteristic of elastic strain is reversibility.” (Findley et al., 1989). More specifically, linear elastic theory is based on the assumption that both the displacement and the displacement gradient are very small. The small nature of the strain is such that there is no necessity to differentiate between LaGrangian and Eulerian coordinate systems. Under this definition, the linear elastic stress-strain relationship can be written as:

\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \]  

(1)

where \( \sigma_{ij} \) is the stress tensor, \( \varepsilon_{km} \) is the strain tensor, and \( C_{ijkl} \) represents 36 distinct elastic coefficients (Lai et al, 1993). The indicial subscripts denote the 3x3 stress or strain components associated with each coordinate axis, representing directional dependence. Likewise, the subscripts on C indicate the directional dependence of stress on strain for the given material. This relationship is referred to as Hooke’s Law, named for the famous English scientist Robert Hooke (1635-1703), the first person to investigate scientifically the elastic properties of materials (Gere, 2006). If a body’s elastic properties, as described by \( C_{ijkl} \), are the same for every orientation of the coordinate axes, then it is said to be an isotropic elastic material (Mase and Mase, 1989). Applying these assumptions to Hooke’s Law (1), yields

\[ \sigma_{ij} = \frac{E}{1+\nu} \left( \varepsilon_{ij} + \frac{\nu}{1-2\nu} \delta_{ij} \varepsilon_{kk} \right) \]  

(2)
where $E$ is the elastic (Young’s) modulus, $\nu$ is Poisson’s ratio, and $\delta$ is the Kroneker delta. Further still, the following pair of terms can be defined.

\[
K = \frac{E}{3(1-2\nu)}
\]  

(3)

\[
G = \frac{E}{2(1+\nu)}
\]  

(4)

$K$ represents the Bulk Modulus, and $G$ represents the Shear Modulus (Findley et al, 1989). Classically, elastic materials are represented, schematically, as a spring (as shown in Figure 2).

![Figure 2 - Spring Element Analog](image)

Viscous Fluids

In stark contrast to elastic solid behavior, fluid behavior is marked by an ability to deform continuously when acted upon by a stress. Fluids, as mentioned earlier, are
classified as either compressible or incompressible. Additionally, fluids are classified as either viscous or invicid. Viscous fluids possess the intrinsic property of viscosity; the ability of the fluid to develop shear stress through its volume. Although no truly invicid fluids exist, it is not uncommon to treat certain fluids as invicid (zero viscosity) when viscous effects are negligible.

The stress-deformation relationship for fluids can be expressed, very generally, as:

\[ \tau_{ij} = f(D) \]  

(5)

where \( \tau_{ij} \) is the shear stress acting on the \( i \) surface in the \( j \) coordinate direction and \( f(D) \) represents a general, undefined function of the deformation rate, \( D \). If the function, \( f \), which describes the fluid is linearly proportional to \( D \), the resulting stress function takes the form:

\[ \tau_{ij} = K_{ijpq}D_{pq} \]  

(6)

\( K \) is a fluid-specific coefficient known as viscosity, frequently reported as \( \eta \). Typically, the strain rate is reported as the time-derivative of strain, which is proportional to the applied stress:
\[ \tau = \eta \frac{\partial \varepsilon}{\partial t} \]  \hspace{1cm} (7)

All fluids which behave in this manner are called Newtonian Fluids, named for Isaac Newton (1643-1727) who investigated this property (Cengel and Cimbala, 2006). This equation (7) simply states that the strain rate is proportional to applied stress. Viscous fluids are classically represented, schematically, as a dashpot, piston, or damper.

![Figure 3 - Dashpot Element Analog](image)

Figure 3 - Dashpot Element Analog

**Linear Visoelasticity**

A combination of Hooke’s Law (2) and Newtonian fluid mechanics (7) leads to linear viscoelastic theory. *Linear* behavior demonstrates the way a material has a constant, linear, relationship between stress and strain. That is to say, the strain exhibited by a material when subjected to a given stress will be exactly doubled when the applied stress is doubled. While most materials are not truly linear in their strain response, material models which attribute linear behavior to such materials are often sufficient. In many cases, materials demonstrate nearly linear behavior over a certain, and usually well-defined, range of stress or strain, beyond which the behavior can be different.
By combining the two models, stress-strain relationships for linear viscoelastic materials can be developed. Two of the simplest applications of this practice are the Maxwell and Kelvin Models.

The Maxwell model consists of a spring and dashpot in series:

\[ \frac{\varepsilon}{G_m} + \frac{\sigma}{\eta_m} = \dot{\varepsilon} \]  \hspace{1cm} (8)

where \( \sigma \) is the stress acting on the pair of elements, \( \varepsilon \) is the resulting strain, \( G \) is the elastic modulus of the spring, \( \eta \) is the viscosity of the dashpot element, and the “dot” indicates a first time derivative (Shames and Cozzaralli, 1997). Indices have been drop
for the one dimensional case. Due to the isolated nature of the dashpot, this model will undergo continuous deformation when subjected to an applied load. For this reason, the Maxwell model is considered to be a viscoelastic \textit{fluid}.

The Kelvin Model, on the other hand, consists of the spring and dashpot elements in parallel:

\[ \sigma = G_k \varepsilon + \eta_k \dot{\varepsilon} \]  \hspace{1cm} (9)

The response of the Kelvin model is drastically different from that of the Maxwell model. The dashpot acts in such away as to dampen the response of the elastic spring element.
Likewise, once the pair is unloaded, the dashpot dampens the recovery of the elastic spring. In a static load condition, the Kelvin model will eventually reach some constant state of strain in which the elastic spring element is carrying the entire load (Shames and Cozzaralli, 1997). For this reason, the Kelvin model is classified as a viscoelastic solid.

Both the Kelvin and Maxwell models have serious limitations in any actual application to describing any real material (Findley et al., 1989). A standard fluid model consists of a Kelvin element and a dashpot, also known as a Jefferies fluid. This simple fluid analog is limited by the fact that it exhibits no immediate elastic response. A similarly simple solid consists of a Kelvin element and a spring. This model will demonstrate time-dependent and instantaneous deformation and recovery, but is limited by the fact that it has no capacity for permanent viscous loss observed in fluids.

The 4-element Burger model consists of a Maxwell and Kelvin element in series.

Figure 6 - Burger fluid model. Kelvin and Maxwell analogs placed in series to make up Burger fluid model analog. An instantaneous response to applied load is exhibited by free spring of Maxwell model and continuous creep is exhibited by free dashpot of...
Maxwell model. The Kelvin model exhibits the same transition between dashpot-dictated creep and long-term spring-dictated displacement as usual.

This model offers the simplest combination of analogs which accounts for instantaneous elastic response, time-dependent deformation and permanent viscous loss. The strain response of this model can be developed by adding the strain response of each of the two models represented in series (Findley et al., 1989).

\[ \tau + \left( \frac{\eta_1}{G_1} + \frac{\eta_2}{G_2} \right) \eta_1 \eta_2 G_1 G_2 \] (10)

As Shown in Figure 6, subscript 1 refers to the serial (i.e. Maxwell) components, and subscript 2 refers to the parallel (i.e. Kelvin) components.

**Creep and Relaxation**

Creep and relaxation are generalized forms of time-dependent behavior as well as common experimental techniques used to clarify or simplify such behavior. Creep is the term used to describe the elongation or shear strain exhibited by a material once subjected to an instantaneously applied and subsequently constant load. If one defines the unit step function, where \( t_1 \) is the time at which said load is applied,

\[ U(t-t_1) = \begin{cases} 0 & \text{if } t \leq t_1 \\ 1 & \text{if } t > t_1 \end{cases} \] (11)
The loading scenario used for a creep situation can be expressed as:

\[
\sigma = \sigma_0 U(t), \quad (12)
\]

where \( \sigma_0 \) is a constant shear, tensile, or compressive stress. A specific shear strain equation for the Burger model can be attained by substituting (12) into the strain response for the Burger model (10) and integrating with respect to time. This procedure yields:

\[
\gamma(t) = \tau_0 \left[ 1 + \frac{t}{\eta_1} + \frac{1}{G_2} \left( 1 - e^{-G_2/\eta_2} \right) \right], \quad (13)
\]

where, \( \gamma \) is the shear strain, and \( \tau_0 \) is the applied constant shear stress. If one considers the effect of removing the applied stress at a specific time, \( t_s \), the behavior of the Burger model in recovery can be described by (Findley et al. 1989)

\[
\gamma(t) = \tau_0 \left[ 1 + \frac{t_s}{\eta_1} + \frac{1}{G_2} \left( 1 - e^{-G_2/\eta_2} \right) \right] - \tau_0 \left[ \frac{t_s}{\eta_1} + \frac{1}{G_2} \left( e^{-G_2/\eta_2} - 1 \right) e^{-G_2/\eta_2} \right]. \quad (14)
\]

The bracketed terms in equations (13) and (14) are defined as the creep compliance of the material. This relationship provides some significant information to the astute observer. First, the Maxwell elastic coefficient can be calculated by the ratio of the applied stress,
\( \tau_0 \), and the instantaneous strain response, \( \gamma(t=0^+) \). Secondly, the Maxwell viscous coefficient can be calculated by taking the product of \( t_s \) and the ratio of the applied stress to the ultimate, unrecoverable strain, \( \gamma(t\to\infty) \). Finally, the coefficients used to describe the Kelvin elements can be calculated by determining the slope of the strain response at \( t = 0^+ \) and \( t = t_s^- \). Since real fluids rarely mimic Burger fluid behavior perfectly, these techniques cannot be expected to give perfectly optimized parameters from experimental results (Findley et al., 1989). They can, however, give very good starting points in the process of optimizing coefficient values to experimental results.

Relaxation is the term given to describe the dissipation of internal stresses in a material under constant strain conditions. In a sense, it is the counter-part to creep. This can be expressed as:

\[
\varepsilon = \varepsilon_0 U(t), \tag{15}
\]

where \( \varepsilon_0 \) is a constant strain, be it compressive, tensile, or shear. In a manner similar to the development of the creep response, equation (9) can lead to the development of the shear creep strain function.

From equations (11) and (12), one can derive a strain history function and its first and second derivative by describing the constant shear strain condition in a fashion similar to constant shear stress:
\[ \varepsilon = \varepsilon_0 U(t); \quad \delta = \varepsilon_0 \delta(t); \quad \delta_\varepsilon = \varepsilon_0 \frac{\partial \delta(t)}{\partial t} \] (16)

Again, \( \varepsilon_0 \) is the constant compressive, tensile or shear strain, and \( \delta(t) \) is the Dirac delta, also known as the Unit Impulse function, having the form:

\[ \delta(t) = 0, \quad t \neq 0; \quad \int_{-\infty}^{\infty} \delta(t) dt = 1. \] (17)

Substituting equation (17) into (16), the 1-dimensional stress-strain relation for a Burger model yields

\[ \tau + \left( \frac{\eta_1}{G_1} + \frac{\eta_2}{G_2} \right) \frac{\partial \tau}{\partial t} + \left( \frac{\eta_1 \eta_2}{G_1 G_2} \right) \frac{\partial^2 \tau}{\partial t^2} = \eta_0 \varepsilon_0 \delta(t) + \left( \frac{\eta_1 \eta_2}{G_1} \right) \varepsilon_0 \frac{\partial \delta(t)}{\partial t}. \] (18)

In order to convert equation (18) into a stress function resembling (13) requires that a Laplace transform be taken. The Laplace transform will provide insight into linear viscoelastic constitutive laws and provide a powerful method for solving the associated stress analysis problems (Shames and Cozzarelli, 1997). The interested reader is directed to any viscoelasticity discussion in an appropriate textbook, such as the one in Creep and Relaxation of Nonlinear Viscoelastic Materials by Findley et al. (1989). The result of applying Laplace transforms is (Findley et al., 1989): \( p, q, \) and \( r \) are simply collected terms to simplify presentation).
\[
\sigma(t) = \frac{e_0}{A} \left[(q_1 - q_2 r_1) e^{-\gamma t} - (q_1 - q_2 r_2) e^{-\gamma t}\right]
\]  

(19)

where

\[
\begin{align*}
  r_1 &= \left( p_1 - A \right) / 2 p_2, \\
  r_2 &= \left( p_1 + A \right) / 2 p_2, \\
  A &= \sqrt{p_1^2 - 4 p_2},
\end{align*}
\]  

(20)

and

\[
\begin{align*}
  p_1 &= \frac{\eta_1 + \eta_2}{G_1}, \\
  p_2 &= \frac{\eta_1 \eta_2}{G_1 G_2}, \\
  q_1 &= \eta_1, \\
  q_2 &= \eta_1 \eta_2.
\end{align*}
\]  

(21)

Collectively, the terms in equation (19), more specifically, their \(G, \eta, G_2\) and \(\eta_2\) combinations defined in the equations given in (20) and (21), are referred to as the shear stress relaxation modulus.

The preceding development of the governing equations of a Burger fluid served to introduce the reader to the form of the relationships required for application in the computer-aided modeling, which will be discussed in Chapter 5, as well as to provide a basis by which parameter values have been determined, by others (Towler, 2004), in laboratory testing. Parameter value determination methods will be discussed further in the next chapter, Chapter 4.
PREVIOUS WORK

Now that the theory of viscoelasticity has been presented, one must consider the validity of using these models to describe the behavior of biofilm when subjected to stresses. Work done by Towler (2004) established that biofilm behaves as a Burger fluid under a discrete range of loadings. Additionally, similar work being conducted by Sutton (2006) confirms the viscoelastic nature of biofilm. While more complex models may provide a more accurate description, the Burger fluid model is the most accurate while remaining relatively simple. Both investigations have carried out extensive rheology work to investigate biofilm material properties.

Rheology

Rheology is the study of the deformation and flow of matter, most typically fluids. More specifically, this field is mostly concerned with non-Newtonian fluids whereas the study of Newtonian fluids is simply referred to as fluid mechanics. Categorizing these materials requires extensive testing.

Both Towler (2004) and Sutton (2006) used a research-grade rheometer (TA Instrument’s AR1000) in the Montana State University Mechanical Engineering Department’s Material Testing Lab. The AR1000 is a disk type rheometer on which the sample is placed between two disks. One disk is stationary (the base) and one is capable of rotating. The rotation applies a controlled stress to the sample while total rotation is recorded, measuring strain.
In Towler (2004) and Towler et al. (2003), biofilm samples were grown in a growth reactor which consisted of three rheometry disks. The biofilm sample was grown on the testing-surface of the disks while submerged in the growth chamber and removed prior to testing. Samples were allowed to grow for 12 days while in the growth reactor. Steps were taken to minimize the effects of changes to the biofilm’s environment during testing, including fashioning a clay barrier around the stationary rheometer base, allowing for the tests to be conducted while the biofilm remained submerged. Biofilm samples were subjected to a constant shear stress for three minutes and the strain response was recorded. Furthermore, the applied stress was removed and the samples were allowed to relax for three additional minutes, all while strain response readings were being recorded.

The results of the above mentioned testing support the claim that biofilm behaves as a viscoelastic Burger fluid. In addition to demonstrating a Burger fluid response, the biofilm exhibited linear viscoelastic behavior. Increasing the applied stress increased the strain response proportionally. Figure 7 shows the strain response of a single biofilm sample subsequently subjected to two different applied loads. First, a 0.1 Pa shear stress was applied for 180 seconds and then removed. After the biofilm sample was allowed approximately 10 minutes for recovery, the sample was subjected to a 0.5 Pa stress for an additional 180 seconds. The results of this procedure were recorded and support the suggestion that biofilm’s strain response to applied stress can be approximated with a linear viscoelastic Burger fluid model (Towler 2004, Towler et al., 2003).
Figure 7 - Strain response of biofilm sample demonstrating linear viscoelastic behavior. A single biofilm sample was subjected to 0.1 Pa stress (3a) for 180 seconds. After allowing a period of recovery, the sample was then subjected to a 0.5 Pa stress (3b) for 180 seconds. The inset shows this loading schedule. The ratio between the two strain curves is denoted with $c$, which is approximately equal to 5, indicating linear viscoelastic behavior. (Towler, 2005)

The time-dependent nature of the response seen in the above data, as well as the whole of the data collected by Towler (2004), clearly indicates that the biofilm exhibited both elastic and viscous behavior. Each curve indicated the material’s capacity for both instantaneous elastic deformation and unlimited deformation, or creep. These characteristics support the classifications made by other investigators (Ohashi and Harada, 1994, Stoodley et al. 1999, 2002, Korstgens et al. 2001a, 2001b, Klapper et al. 2002) of biofilm as a viscoelastic material; this time, it was done through the use of an accepted material testing technique (Towler, 2004).
Previous In Situ Testing

Stoodley et al. (1999, 2002) developed an experimental technique for testing the response of biofilm to turbulent flow conditions. Microbial biofilm was grown in glass flow-through cells under varying conditions. Individual biofilm colonies were identified and, using digital time lapse microscopy (DTLM), measurements of elongation versus changes in average flow rates were taken. In the absence of a better estimate, these studies used the calculated theoretical wall shear for a smooth pipe as the representative stress acting on the biofilm cluster. These experiments demonstrated the viscoelastic nature of biofilm. The claim made by these investigators that these in situ tests were “analogous to stress-strain and creep tests on attached biofilms” is optimistic. Stress-strain tests are well-defined and highly controlled procedures involving the application of a prescribed or measurable load to a material. The response of the material is measured in a similarly fastidious manner. In these investigations by Stoodley et al. (1999, 2002), biofilm was observed to have deformed, and to have crept in response to the fluid-induced forces, but neither the forces nor the deformations were measured with the accuracy that stress-strain and creep testing allow. The actual applied forces are complex, three-dimensional forces varying spatially, not a single value, unidirectional force. Despite these criticisms, measuring the local velocity distributions and resultant forces empirically would have been difficult and problematic. A computational simulation of this type of biofilm-fluid interplay would eliminate the need to attempt to measure the local velocities and deformations and provide a tool to be used in further investigations into the response of biofilm to fluid flow.
Two-Dimensional Model

Along with the extensive material testing mentioned earlier, Towler et al. (2006) developed a two-dimensional fluid-solid finite element model (FEM) based on the geometry of the work done by Stoodley et al., (1999, 2002) to which the results of the rheometry testing were applied. The model mimics the setup of the work done by Stoodley et al. (1999) by replicating the 2 mm channel size. Towler employed ANSYS 7.1, a widely-used finite element modeling software package, to model the interaction of biofilm with flowing fluid. Utilizing ANSYS’ fluid-solid interaction (FSI) capability, the investigator was able to model, in two dimensions, biofilm creep and relaxation as a result of fluid-induced stresses by defining a biofilm material which was attached to the fluid boundary. The model represented biofilm geometry as a square and a semi-circle. This model provided a good compliment to the work of Stoodley et al. (1999, 2002), providing more detailed descriptions of the local fluid velocities and induced stresses. The computational model was then employed in a extensive parametric study in order to examine the behavior of biofilm. Variations were made to each of the four Burger fluid parameters, $G_1$, $\eta_1$, $G_2$, and $\eta_2$, to investigate their respective influence on the response. Furthermore, channel fluid velocity was varied, and the results to biofilm behavior were documented.

As mentioned previously, limitations in the measurement of local fluid forces around biofilm colonies led Stoodley et al. (1999, 2002) to simplify models of fluid-caused forces on the biofilm. With respect to Towler (2004), a two dimensional model could certainly be improved with inclusion of a third dimension. A two-dimensional
computational model allows one to much more closely monitor fluid flow and fluid-induced stresses and the resulting behavior exhibited by the biofilm. Such a model is a vast improvement upon the assumption that theoretical wall shear stress is representative of the complex hydrodynamic conditions that exist around a body protruding into a flowing stream of water, especially a non-rigid body which interacts dynamically with the flow. Clearly, a three dimensional model will bring the process one step closer to replicating biofilm behavior. It would also prove beneficial to develop a model of biofilm which allows for additional complexity in geometry, thereby more closely mimicking actual biofilm clusters.

Armed with the information gleaned by Stoodley et al. (1999, 2002) and Towler et al. (2006), as well as a three dimensional FSI biofilm model, additional simulations were undertaken in order to quantify both adhesive and cohesive stresses in biofilm clusters. Such knowledge will provide a better understanding of the mechanisms which must be employed to better predict biofilm detachment, as well as help in identifying key biological morphologic behavior that impair hydrodynamic efficiency in closed-conduit systems.
DEVELOPMENT OF THREE-DIMENSIONAL COMPUTATIONAL MODEL

In previous sections, the experimental work done by Stoodley et al. (1999) and Towler et al. (2003) were presented to justify the applicability of the linear elastic Burger model for representing the deformation of a biofilm cluster when subjected to external forces. This stress-strain relationship has been applied to a three-dimensional computational model.

Problem Description

Using the configuration which Stoodley et al. (1999) as a basis, a Finite Element Model (FEM) representing the Fluid-Solid Interaction (FSI) between biofilm and fluid flow was developed in the interest of simulating the biofilm cluster response to turbulent flow conditions. The ANSYS software mentioned earlier was the platform for the development of the numerical model.

FEM Platform

ANSYS version 8.1 is a widely used finite element program which utilizes numerical methods and the power of modern computers to solve equations of motion and state for both solid and fluid materials and is capable of being used to solve thermal, structural, electro-magnetic, and fluid problems. It is a self-contained program which has a comprehensive graphical user interface (GUI) that gives users easy, interactive access to program functions and commands. Additionally, users can define problem parameters and solution methods to a very high level of specificity with the ANSYS Parametric
Design Language (APDL). ANSYS is capable of coupled-field analyses in which two material realms can interact realistically allowing for users to model the interactions between flowing fluid and a deformable object which protrudes into the flow stream.

**Solid Mechanics in ANSYS**

The partial differential equations which govern strain deformation can be developed through the principle of virtual work (ANSYS, Inc., 2004). The method which ANSYS uses in its FEM divides the domain to be solved into several sub-regions called elements. Solutions to the differential equations for each element are developed while maintaining continuity at element boundaries. Element boundary conditions may be domain boundary conditions, or the conditions of the adjacent element. By satisfying prescribed domain boundary conditions (e.g. specified loads, displacement constraints) and inter-element continuity, material constitutive laws can be used to solve a well-defined solid mechanics problem.

Boundary conditions describe known conditions at a domain’s boundary, and are specific to any given problem. For a biofilm cluster, the only constant boundary condition is that it is attached to a stationary substratum. The boundary conditions existing on the remaining surfaces of the biofilm are the hydrostatic and hydrodynamic loads. The loads exerted on the biofilm by the fluid are, clearly, not known prior to solving the model. This is precisely why a coupled field analysis is needed. This allows the loads developed by the fluid to be coupled to the biofilm’s non-stationary surfaces. This, however, requires that the fluid solution must be completed to derive those loads.
This solution procedure is called a sequentially coupled analysis due to the sequence of solution and load transfer.

**Burger Model in ANSYS**

The Burger model, as previously presented, was used to relate stress and strain in the ANSYS model. The representation of the Burger model needed to be adapted to a format suitable for ANSYS. Non-linear material behavior can be incorporated into ANSYS in a number of different ways. ANSYS supports many different element types, each with its own strong points. With this in mind, it is important that elements used in any given analysis meet the requirements imposed on it by the given scenario. Performing a viscoelastic coupled field analysis required that element types used supported both fluid and structural types of analysis, and that the structural elements used to represent the biofilm were compatible with a viscoelastic material description. This necessitated the use of the SOLID18X family of elements. This family is three dimensional structural elements that permit non linear strain response through the use of a Prony series and application of coupled-field loads, making it a good choice for the biofilm model. SOLID185 is an eight node hexahedron; there are nodes at each vertex. SOLID185 was used in the biofilm model.

A Prony series allows a viscoelastic, time-dependent material response to be represented in ANSYS in the following form (ANSYS, Inc., 2004)

\[ C(t) = C_0 + \sum_{i=1}^{k} C_i e^{-\alpha_i t}, \]  

(22)
where \( t \) is time, \( a_i \) are the \( k \) exponential Prony coefficients and \( C_i \) are the \( k+1 \) linear Prony coefficients. The subscript \( i \) indicates the number of a given term, up to the maximum, \( k \). In the case of a Burger fluid expressed as a Prony series, \( k = 2 \). Equation (22) is of the same form as the relaxation function for a generalized Maxwell model, (Findley et al. 1989) which is:

\[
G(t) = G_1 e^{-t/\tau_1} + G_2 e^{-t/\tau_2} + K + G_{n-1} e^{-t/\tau_{n-1}} + G_n e^{-t/\tau_n},
\]

(23)

where \( G_1 \) through \( G_n \) are the shear moduli and \( \tau_1 \) through \( \tau_n \) are the relaxation moduli for the \( n \) Maxwell units in parallel. Equating equations (22) and (23) with \( n = k = 2 \) results in a Prony series representing two parallel Maxwell models. That is to say, a four element general Maxwell model:

\[
C(t) = G_m + \sum_{i=1}^{n} G_i e^{-t/\tau_i} \quad n = 2.
\]

(24)

In the above form, \( G_m \) is representative of the shear modulus at \( t = \infty \). Based upon the evidence presented earlier (Stoodley et al. 1999, Towler 2004, Sutton 2006) that biofilm behaves as a viscoelastic fluid, the residual shear stresses at \( t = \infty \) must be zero. This allows \( G_m \) to be neglected, resulting in
This development shows that any general Maxwell model can be easily represented in a Prony series. A four element Burger model presents a more complex case. As outlined in Chapter 3, a Laplace transform is utilized, yielding the following as the Burger relaxation Modulus

\[ G(t) = G_1 e^{-\frac{t}{\tau_1}} + G_2 e^{-\frac{t}{\tau_2}}. \] (25)

\[ G(t) = \frac{n_1 - \eta_1 \eta_2 T_1}{G_2} \frac{e^{-r_1 t}}{\sqrt{\left(\frac{n_1 + n_1 + n_2}{G_1} + \frac{n_2}{G_2}\right)^2}} - \frac{-\left(\frac{n_1 - \eta_1 \eta_2 T_2}{G_2}\right)}{\sqrt{\left(\frac{n_1 + n_1 + n_2}{G_1} + \frac{n_2}{G_2}\right)^2}} - 4 \frac{\eta_1 \eta_2}{G_1 G_2} } e^{-t_2 t} \] (26)

where \( T_1 \) and \( T_2 \) are

\[ T_1 = \frac{n_1 + n_1 + n_2 - \sqrt{\left(\frac{n_1 + n_1 + n_2}{G_1} + \frac{n_2}{G_2}\right)^2}}{G_2} \] (27)

\[ T_2 = \frac{n_1 + n_1 + n_2 + 2 \frac{\eta_1 \eta_2}{G_1 G_2} \left(\frac{n_1 + n_1 + n_2}{G_1} + \frac{n_2}{G_2}\right)^2} {\frac{2 \eta_1 \eta_2}{G_1 G_2}} \] (28)
These terms define the coefficients to be used in equation (22) to define the Prony series for a Burger fluid. That is to say

\[
C_1 = \frac{\eta_1 - \eta_1 \eta_2}{G_2} \left[ \left( \frac{\eta_1}{G_1} + \frac{\eta_1}{G_2} + \frac{\eta_2}{G_2} \right)^2 - 4 \frac{\eta_1 \eta_2}{G_1 G_2} \right] - 4 \frac{\eta_1 \eta_2}{G_1 G_2}
\]

\[
C_2 = \frac{-\eta_1 + \eta_1 \eta_2}{G_2} \left[ \left( \frac{\eta_1}{G_1} + \frac{\eta_1}{G_2} + \frac{\eta_2}{G_2} \right)^2 - 4 \frac{\eta_1 \eta_2}{G_1 G_2} \right] - 4 \frac{\eta_1 \eta_2}{G_1 G_2}
\]

\[
a_i = \frac{\eta_i + \eta_1 + \eta_2}{G_1 G_2} \left[ \left( \frac{\eta_1}{G_1} + \frac{\eta_1}{G_2} + \frac{\eta_2}{G_2} \right)^2 - 4 \frac{\eta_1 \eta_2}{G_1 G_2} \right] - 4 \frac{\eta_1 \eta_2}{G_1 G_2}
\]
The coefficients defined in equations (29-32) were calculated through ADPL statements in the ANSYS input file using the user-defined Burger coefficients \( G_1, G_2, \eta_1 \) and \( \eta_2 \), thus allowing ANSYS SOLID185 to represent a Burger fluid in the analysis.

\[
a_2 = \frac{\eta_1}{G_1} + \frac{\eta_1}{G_2} + \frac{\eta_2}{G_2} + \sqrt{\left(\frac{\eta_1}{G_1} + \frac{\eta_1}{G_2} + \frac{\eta_2}{G_2}\right)^2 - 4 \frac{\eta_1\eta_2}{G_1G_2}}
\]

\[ (32) \]

Fluid Dynamics in ANSYS

ANSYS 8.1 uses FLOTRAN for computational fluid dynamics (CFD). ANSYS structural solutions and FLOTRAN CFD solutions both utilize finite element techniques, but they differ in their execution. Fluid regions are divided into elements in the same manner as structural regions. The Navier-Stokes equations as well as, when appropriate, a turbulence model are assembled to complete the FEM solution. The final solution is reached through an iterative process in which residual changes are monitored and, once residual changes are satisfactorily small, the solution is considered “converged.” Multiple fluid solvers are available in FLOTRAN, as well as numerous turbulence models. All solution methods are based on the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) technique developed by Patankar (1972).

As with solving differential equations or simple numerical solutions, boundary or initial conditions must be defined in CFD problems. In the case of the numerical simulation performed, velocity was defined at the inlet of the flow channel and pressure...
was defined at the flow region outlet. Additionally, no-slip and zero-displacement conditions were specified along the flow boundaries. The solution for pressure and shear stress at the biofilm interfaces are used as loads which are transferred to the biofilm structure through the FSI load coupling process.

**Fluid-Structure Interaction**

A fluid-structure interaction analysis is carried out in ANSYS by creating two separate models, each governed by a specific set of material properties, and then coupling them across a defined interface. Coupling describes the process by which the solutions to the two different models are linked. An interface can be any similar or dissimilar mesh boundary between the two models. ANSYS uses a sequential coupling algorithm. The first step in the process which ANSYS uses to solve coupled models is to solve the fluid realm first, then apply the boundary loads (pressure and shear forces) to the biofilm region. This process is carried out numerous times depending on the total time of simulation as well as the time step. Once the solid solution has converged, the fluid region is updated to reflect the new geometry of the solid. Then, the next fluid solution is determined, hence the “sequentially coupled” moniker. The process can be conceptualized in a figure, shown below.
Figure 8 – Weakly coupled ANSYS FSI algorithm. Stagger loop iterates until convergence criteria is met. Once convergence criteria are achieved, solution advances through time loop (ANSYS, Inc., 2004)

Model Geometry and Geometric Parameters

The model was built to the same geometry as the experimental setup in Stoodley et al. (1999, 2002). The flow channel was 3 mm in height as well as width. Channel length was 200 mm. A biofilm consisting of nine (3x3) square bases was located at the center of the channel bottom (in the X-Y plane at the coordinate origin). The sizes of the blocks were user-definable. 100 μm biofilm block size was simulated, resulting in a cluster with a square footprint of 300 μm per side. The heights of the biofilm blocks were also user-definable. In the interest of making the biofilm top surface continuous
and consisting of only planar areas, not all height dimensions were independent. Figures 9 and 10 below show the model’s geometric layout as well as some examples of the geometric possibilities for the biofilm.

Figure 9 – Biofilm flow channel. Biofilm location is centered at the coordinate origin. Channel length is 200 mm. The volume regions in the center of the channel are a result of the careful meshing procedures used in defining the finite element divisions for solving the problem.
Figure 10 – Three different biofilm geometry examples to show the possibilities for biofilm shape. The 9 volumes shown would be divided into elements for solution of the problem.

In addition to biofilm geometry, the mean flow velocities, as well as the Kelvin and Maxwell material model parameters were variables which could be defined by the user.

In any FEM, the fineness and distribution of the mesh which defines the elements is very important. In the three-dimensional FSI biofilm model, the mesh was finest near the biofilm where fluid flow was most affected by the biofilm and, as a result, special gradients of the flow field were highest. In the entrance and exit regions, fewer elements were used in the interest of reducing the total number of elements and speeding the solution process. Mesh divisions were defined in the ADPL and can be altered to increase speed or accuracy. The mesh pattern used showed sufficient accuracy. Solution results did not improve noticeably with increased mesh fineness, and solution times were reasonable. In addition to these mesh constraints, the ANSYS education version which was used has a limited number of elements. Specifically, 512,000 elements is the maximum allowed in the ANSYS educational version which was used (ANSYS, Inc.,
Ultimately, mesh fineness was limited by the version of ANSYS which was used. Figure 12 below shows the meshed fluid channel.

![Meshed fluid channel](image)

Figure 11 – Meshed fluid channel. Biofilm base is on the low-Z (close) side, at the origin.

After establishing a workable mesh, and running a number of simulations to determine reasonable material property values, parametric studies were defined and carried out.
SIMULATIONS

With the groundwork laid on the application of the Burger model to ANSYS, these FSI models were put to use. The model could shed light onto fluid-force induced biofilm behavior phenomena which has been the subject of many previous investigations.

Background on Burger Application

In the work done by Stoodley et al. (1999), mentioned in earlier chapters, investigations into the structural deformation of biofilms caused by fluctuations in fluid shear were made. Stoodley et al. (1999) suggested that changes in biofilm shape will affect the hydrodynamic drag which in turn will influence the detachment rate and pressure losses in a flowing system. The method used to correlate fluid shear to biofilm colony deformation, however, was not able to address the possibility of drag forces changing as the biofilm shape changed. The characteristic stress assumed to be acting on the biofilm was taken to be the mean wall shear stress acting on a theoretically clean channel boundary of equivalent geometry to that in the experimental setup (Stoodley et al., 1999). Measuring the fluid forces acting on the biofilm would have been difficult. Thus, changes in drag forces were not able to be documented. As mentioned before, not measuring the actual applied stress on the biofilm was less an exclusion than an impossibility. With the three dimensional FSI numerical model however, changes in the drag force acting on the biofilm could be tracked.

A starting point for a parametric series was needed. Based upon the methods used in the work done by Stoodley et al. (1999), the angle along the leading edge of the
biofilm cluster varied by approximately ten degrees through the experiments conducted. In this series of experiments the Reynolds number ranged from 0 to 432. Starting-point values for the Maxwell and Kelvin parameters were taken to approximate this range of deformation. While the biofilm cluster observed by Stoodley et al. (1999) was clearly not a cube, the simplified geometry of a cube was used for these parametric studies. The geometry of real biofilm structures is highly complex. Often, the complexity of biofilm can hide results which might more readily be observed with a more simple shape. For this reason, a cube was used for its simplicity to elucidate the fluid-structure interaction and material behavior. Further simulations could be run with geometry which specifically mimics any given biofilm cluster.

Parametric Study of Burger Fluid Parameters’ Effect on Drag Force

A series of simulations was created to investigate the relationship between the material model coefficients and the time-dependent fluid drag forces acting on the biofilm. It was determined that the baseline parameter values used by Towler (2004) in his two dimensional model were appropriate in matching the leading edge angle deflection observed by Stoodley et al. (1999). The baseline set of parameter values are the “central” set, and are associated with any series ending with the number 5. Series ending with values less than 5 suggest that the varied parameter(s) were less than the value in the baseline series, and series ending with values greater than 5 suggest that the varied parameter(s) were greater than the value in the baseline series. Each series was comprised of 9 parameter sets. In all, 4 parameter sets were varied, resulting in 36
different parameter combinations. In addition, the set of 36 different parameter combinations was reproduced in triplicate under three different fluid velocity values.

The goal of the parametric series was to correlate the effects of biofilm material properties to the fluid-induced drag force acting on the biofilm and investigate the potential role that biofilm material properties play in detachment potential or survivability. As with Towler’s (2004) work, the parameter values were varied in the interest of producing a wide range of deformations. In each series, a single parameter was varied to achieve a given strain ratio with the baseline set. The Series tables below include the strain ratios for each simulation. In the work done by Stoodley et al. (1999), biofilm samples were observed with constant flow rates for 30 seconds. The duration of the initial simulations was held constant at 30 seconds, with load transfer in the FSI model taking place at 5 seconds in order to closely match the time scale used by Stoodley. Additional simulations were also run once the results of the initial series were complete to investigate the results over longer time scales. A sample ADPL input file of simulation 05 is included in Appendix A.

**Series 0: Maxwell Elastic Modulus Varied.** In Series 0, the Maxwell elastic modulus, $G_1$, was varied. The relaxation time of the Maxwell element was held constant, resulting in variations in $\eta_1$. Table 2 lists the parameter sets investigated.
Table 1 – Series 0 material model coefficient values. Vary $G_1$ while holding $T_1$ constant.

<table>
<thead>
<tr>
<th>Series</th>
<th>Units</th>
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<th>02</th>
<th>03</th>
<th>04</th>
<th>05</th>
<th>06</th>
<th>07</th>
<th>08</th>
<th>09</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_1$</td>
<td>kg/mm-s$^2$</td>
<td>1.77</td>
<td>2.22</td>
<td>3</td>
<td>4.62</td>
<td>10</td>
<td>13.04</td>
<td>18.74</td>
<td>33.31</td>
<td>149.26</td>
</tr>
<tr>
<td>$\eta_1$</td>
<td>kg/mm-s$^2$</td>
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<td>33.3</td>
<td>45</td>
<td>69.3</td>
<td>150</td>
<td>195.6</td>
<td>281.1</td>
<td>499.65</td>
<td>2238.9</td>
</tr>
<tr>
<td>$T_1$</td>
<td>s</td>
<td>15</td>
<td>15</td>
<td>15</td>
<td>15</td>
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<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>$\eta_2$</td>
<td>kg/mm-s$^2$</td>
<td>100</td>
<td>100</td>
<td>100</td>
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<td>100</td>
</tr>
<tr>
<td>$T_2$</td>
<td>s</td>
<td>5</td>
<td>5</td>
<td>5</td>
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</tr>
<tr>
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<td>4.0</td>
<td>3.0</td>
<td>2.0</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Series 1, 2, and 3 deformed such that the solution was not able to converge. The lower set numbers represent biofilm structures with the lowest Maxwell elastic modulus and viscous coefficients. The low Maxwell material coefficients allow excessive deformation, leading to convergence failure. Inspection of ANSYS output and error files indicated that excessive deformation of the biofilm cluster resulted in some elements become inverted. Such inversion, indicated by a zero or negative volume error in ANSYS, prevents the simulation from continuing. The deformations in sets 01-03 were great enough to cause the elements down stream of the biofilm to experience this inversion of space, resulting in convergence failure. Sets 04-09 converged successfully.

The fluid-induced pressure and shear forces acted upon the biofilm structure, resulting in biofilm deformation. Internal stresses developed in the biofilm as a result of these applied loads. Before the FSI loads were applied, the biofilm existed in a zero-stress state as seen in Figure 13. Once fluid loads were applied to the biofilm, however, the stress state reflected the applied loads, as seen in Figure 14, which depicts the stress state at the end of the 30-second simulation. In both figures, flow direction is left to
right, and perpendicular to the left-facing surface. Stresses plotted in Figure 14 are von Mises stresses. Von Mises stress is a frequently used representation of stress intensity in two and three dimensions. The von Mises stress is expressed as:

$$\sigma_v = \sqrt{\frac{(\sigma_1 - \sigma_2) + (\sigma_2 - \sigma_3) + (\sigma_3 - \sigma_1)}{2}}$$  \hspace{1cm} (33)$$

where \( \sigma_1, \sigma_2 \) and \( \sigma_3 \) are the principal stresses. A maximum stress (at the end of the 30-second simulation) of 0.762 mN was recorded at the top of the trialing edge of the biofilm. A vector plot of the flow field around the biofilm cluster is also presented in Figure 14.
Figure 12 – Initial geometry and stress state of simulation 05. The material is not loaded and is unstressed.
Figure 13 – Final Geometry and stress state of simulation 05. At t = 30 seconds, the material has been loaded for 25 seconds. Contours represent internal von Mises stresses (mN). The maximum stress is indicated by the MX, and is located at the top center of the trailing edge.
Figure 14 – Flow path around biofilm structure. Units are mm/s. Note the velocity pattern on the downstream side of the biofilm where flow direction is reversed. Mean channel velocity was 1000 mm/s. Using the channel height as the characteristic length, the resulting Reynolds Number was 3000.

The shape of the biofilm changed with time in response to the pressure and shear forces. The center of the top surface of the biofilm was tracked with respect to x-direction movement through the course of the simulation. The top center point was chosen as a fiducial due to the fact that the displacement of the upper surface would be most influenced by increasing drag forces. The effect of tracking said point allowed the
effects of the drag forces to be elucidated. Figure 15 shows the displacement of the fiducial point for each set.

Figure 15 – Series 0X showing the displacement of biofilm’s top planiform centroid. Maxwell coefficients increase from Series 01 to Series 09. Start of FSI is indicated as well as relaxation time of Kelvin component. The Kelvin relaxation time has physical meaning for constant loads. As seen in Figure 16, applied loads do not remain constant. Consequently, there is no constant transition time between Kelvin and Maxwell behavior.

As the geometry of the biofilm changed, the resulting drag force (X-direction) was monitored. Figure 16 shows the resulting variations in drag forces acting on the biofilm structures represented in series 0X. Series 01-03 are shown in both Figure 16 and 17, but only during the portion of the run where the solution was valid (i.e. before it failed to converge.) The horizontal line on the graph in Figure 17, labeled “SS FX”,

indicates the steady-state force which would act on a rigid cube. It is given as a reference force for comparison to the forces acting on the deformable biofilm.

![Series 0X](image)

**Figure 16** – Series 0X showing change in x-component of resultant fluid force through time. Maxwell component parameter values decrease from Series 01 – Series 09. Solid black line indicates the steady-state drag force acting on a solid cube. Note variation (and increase) in drag force once fluid forces are applied at 5 seconds.

The resultant force in the x-direction is positive throughout the duration of the experiment but is reduced immediately after the fluid forces are applied to the biofilm and increases as the biofilm deforms. The drag force increased for biofilms with lower values of $G_1$ and $\eta_1$, exposing more surface area to fluid shear interactions as well as permitting more stretch of the biofilm, placing it further into the velocity profile,
resulting in increased momentum transfer. Thus, a softer biofilm was subjected to a greater drag force. The action of the fluid-induced deformation through drag forces subjected the biofilm to increasing forces, magnifying the deformation and, eventually, leading to a non-converging model.

**Series 1: Kelvin Elastic Modulus Varied.** In series 1, the value of the Kelvin elastic modulus $G_2$ was varied. As with series 0, the relaxation time was held constant. Accordingly, the Kelvin viscous coefficient, $\eta_2$ changed in response to $G_2$. Table 2 shows the parametric values.

Table 2 – Series 1 material model parameter values. Vary $G_2$ while holding $\tau_2$ constant.

<table>
<thead>
<tr>
<th>Series</th>
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<th>19</th>
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</thead>
<tbody>
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<td>10</td>
<td>10</td>
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<tr>
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<td>42.2</td>
<td>67.1</td>
</tr>
<tr>
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<td>kg/mm-s</td>
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<td>154</td>
<td>211</td>
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<td>5</td>
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<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
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</tbody>
</table>

In Series 1, all nine simulations converged due to the fact that displacements were not as great as in Series 0. Due to the reduced displacement, none of the simulations encountered the negative volume element problems associated with sets 01-03 in Series 0.

In response to the applied fluid load, again at $t = 5$ seconds, not all samples showed an immediate reduction in drag force. In sets 11-13 the drag force increased as
soon as the fluid forces were applied, suggesting that the biofilm deformed very quickly. Additionally, each sample showed that a constantly increasing drag force existed approximately 5 seconds after the fluid forces were applied. The fact that all samples showed the same rate of increase in drag force can be attributed to the fact that $\eta_1$ was the same for each set. The relaxation time for the Kelvin model in each set was held constant at a value of 5 seconds. While the amount of deformation that took place after fluid forces were applied varied from set to set, the time over which the transition from Kelvin-dominated behavior to Maxwell-dominated behavior remained constant at 5 seconds. Since each set had identical Maxwell coefficients, and the applied drag force didn’t vary as much as in Series 0 (compare Figure 16 to Figure 18, noting different y-axis scales), long-term fluid behavior is demonstrated by constant and similar displacement rates after 5 seconds. Displacement of the biofilm is represented in Figure 18. This can be seen in Figure 19 by noticing that at $t = 10$ seconds, the slope of the drag force for each set reaches a steady value. The fact that the drag force continued to increase agrees with the fluid description being used. That is, when $t \rightarrow \infty$, the deformation, and therefore the drag force, will, theoretically, also tend toward infinity. In reality, the biofilm would have detached long before any such occurrence. The deformation results in Series 1 match the form of the results obtained by Stoodley et al. (1999, 2002) using *in-situ* experiments.
Figure 17 – Series 1X. Displacement of biofilm’s top planiform centroid is shown. Kelvin material parameters are varied. Notice influence on total displacement. Near steady-state continuous flow reflects like values between all Maxwell viscous parameters.
Figure 18 – Series 1X. Changes in x-component of fluid force through time are shown. Larger deflections indicated in Figure 17 are correlated with increasing drag forces indicated above.

**Series 2: Maxwell Elastic Modulus Varied.** In Series 2, the value of the Maxwell elastic modulus, $G_i$, was varied again. In contrast to Series 0, however, the viscous coefficient, $\eta_1$, was held constant. This resulted in the Maxwell relaxation time, $\tau_1$, varying in response to changes in $G_i$. Table 3 lists the parameter sets used in Series 2.
Table 3 – Series 2 material model parameter values.

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<th>Series</th>
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<th>23</th>
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<td>2.22</td>
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<td>21.04</td>
<td>33.31</td>
</tr>
<tr>
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<td>kg/mm-s</td>
<td>150</td>
<td>150</td>
<td>150</td>
<td>150</td>
<td>150</td>
<td>150</td>
<td>150</td>
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<td>150</td>
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<tr>
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<tr>
<td>$\eta_2$</td>
<td>kg/mm-s</td>
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<td>100</td>
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<td>5.0</td>
<td>4.0</td>
<td>3.0</td>
<td>2.0</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
</tr>
</tbody>
</table>

As with Series 1, displacements were not large enough to result in negative volumes, but the results of Series 2 are a bit surprising. Series 2 was the only series in which drag force decreased and remained that way. The fact that $\eta_1$ was held constant, allowing the relaxation time of the Maxwell element to vary played an important role in this behavior. For series 21-24, the relaxation time of the Maxwell element exceeded the duration of the simulation. Based on other results, it is likely that the long-term effects of fluid-induced forces would result in an increasing drag force even on Sets 21-24. As the results of the displacement plot indicate, the relatively small elastic modulus for the Maxwell component, $G_1$, resulted in significant deformation oscillations. Recalling that $G_1$ represents the free, undamped spring, large displacements will be realized instantaneously due to the load application. Analogous to releasing a large mass on a soft spring, deformations were large and had a tendency to overshoot steady-state values, resulting in convergence failure. This behavior can be seen particularly well in set 21 in Figure 20.
Figure 19 – Series 2X. Displacement of biofilm’s top platform centroid is shown. Small values of $G_f$ resulted in instability, reflected in the oscillatory behavior, and eventual termination, in Series 21.
Series 2X. Change in x-component of fluid force through time is shown. Smaller deflections in most of the simulations, as shown in Figure 19, resulted in smaller changes in drag force.

Series 3: Kelvin Elastic Modulus Varied. The value of the Kelvin elastic modulus, $G_2$, was varied as in Series 1. In the case of Series 3, however, the viscous coefficient, $\eta_2$, was held constant, resulting in variations in the Kelvin relaxation time, $\tau_2$. Table 4 lists the parameter sets investigated in Series 3. The result of varying Kelvin relaxation time can be seen in the displacement as well as the drag force in the form of
the different times taken to before demonstrating viscous flow behavior by the displacement and drag force. This can be seen in Figures 22 and 23.

Table 4 – Series 3 material model parameter values.

<table>
<thead>
<tr>
<th>Series</th>
<th>Units</th>
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<th>32</th>
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<td>10</td>
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</tr>
<tr>
<td>$\eta_1$</td>
<td>kg/mm-s</td>
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<td>150</td>
<td>150</td>
<td>150</td>
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<td>30.88</td>
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<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.2</td>
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</table>

Figure 21 – Series 3X. Displacement of biofilm’s top planiform centroid is shown. Although varying loads obscure relaxation time behavior, the general trend of increasing relaxation time can be seen.
Figure 22 – Series 3X. Change in x-component of fluid force through time is shown. Variation in the Kelvin spring parameter resulted in changes in relaxation time. Near steady-state drag force increases are similar, resulting from constant values for Maxwell viscous parameter.

Additional Series Results with Variations in Flow Velocity

In addition to Series 0-3, simulations were run with varying flow rates. In Series 10-13, the viscoelastic Burger model parameters were the same as in Series 0-3, but the mean channel velocity was decreased from 1000 mm/s to 750 mm/s. In a similar manner, Series 20-23 have the same viscoelastic model parameters; the mean channel velocity, however, was increased to 1250 mm/s. The resulting Reynolds number for Series 0, 10,
and 20 were 2250, 3000, and 3750, respectively. Graphs showing the drag force acting on the biofilm structure for Series 10-13 and 20-23 are given in Figures 24-31.

**Figure 23 – Series 10X.** Change in x-component of fluid force. Model parameters are the same as in Series 0X, but fluid channel velocity has been reduced to 750 mm/s.

**Figure 24 – Series 11X.** Change in x-component of fluid force. Model parameters are the same as in Series 1X, but fluid channel velocity has been reduced to 750 mm/s.
Figure 25 – Series 12X. Change in x-component of fluid force. Model parameters are the same as in Series 2X, but fluid channel velocity has been reduced to 750 mm/s.

Figure 26 – Series 13X. Change in x-component of fluid force. Model parameters are the same as in Series 3X, but fluid channel velocity has been reduced to 750 mm/s.
Figure 27 – Series 20X. Change in x-component of fluid force. Model parameters are the same as in Series 0X, but fluid channel velocity has been increased to 1250 mm/s.

Figure 28 – Series 21X. Change in x-component of fluid force. Model parameters are the same as in Series 1X, but fluid channel velocity has been increased to 1250 mm/s.
Figure 29 – Series 22X. Change in x-component of fluid force. Model parameters are the same as in Series 2X, but fluid channel velocity has been increased to 1250 mm/s.

Figure 30 – Series 23X. Change in x-component of fluid force. Model parameters are the same as in Series 3X, but fluid channel velocity has been increased to 1250 mm/s.
It was noted that although the magnitude of the drag force changed as a result of differing channel velocities, the form of the response remained consistent between series with identical material law coefficients.

**Motivation for Additional Series**

After observing the effects of changes in material law coefficients, as well as changes in velocity, and noticing the tendency of the displacement and drag force to work together to magnify and accelerate the deformation rate, additional Series were identified and run to investigate the same effects over longer time periods. Of particular interest was the identification of microbial generation times, the time it takes for binary fission to occur for a given microbial species, and comparison to drag and deformation over that generation time scale.

Observations made by Stoodley et al. (1999, 2002), Towler (2004), Klapper et al. (2002), and Sutton (2006) report biofilm stress response behavior in light of short stress application times, ranging from less than one minute to three minutes. Over this short time scale, biofilm exhibited viscoelastic fluid behavior, as noted in previous sections. It is clear that biofilm is able to remain on pipe walls during constant fluid flow. If biofilm behaves as a viscoelastic fluid for large time scales, it would be impossible for it to remain on the pipe wall. One likely explanation for this disconnect between observed biofilm persistence and exhibited stress response is the simple fact that biofilm is not a static conglomeration of parts but is an amalgamation of inanimate bits and living
organisms. The dynamic nature of biofilm necessitates that any stress response be considered in light of the time period over which it is observed.

The time it takes for a given microbial species to undergo binary fission, or reproduce, is called generation time. Generation time is specific to each microbial species, but is generally between 0.3 and 1.5 hours for common biofilm constituent species and is dependent on specific environmental conditions such as temperature, and the amount and type of nutrient (Characklis et al., 1990). Table 5 indicates the approximate generation times for several microbial species under plentiful nutrient conditions.

Table 5 – Generation times for several common biofilm species (Characklis et al., 1990).

<table>
<thead>
<tr>
<th>Species</th>
<th>Generation Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Bacillus mycoides</em></td>
<td>0.5</td>
</tr>
<tr>
<td><em>Bacillus thermophylus</em></td>
<td>0.3</td>
</tr>
<tr>
<td><em>Escherichia coli</em></td>
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</tr>
<tr>
<td><em>Staphylococcus aureus</em></td>
<td>0.5</td>
</tr>
<tr>
<td><em>Pseudomonas aeruginosa</em></td>
<td>1.5</td>
</tr>
</tbody>
</table>

Once the time scale for deformation observation reaches the time scale of generation time, it is no longer reasonable to assume that the material properties of a given biofilm cluster have remained constant. Considering that microbial processes other than fission are also taking place on the same time scale, it is reasonable to assume that biofilm material properties are capable of changing over time scales that match the generation time. One specific process which occurs in microbial colonies is the generation of EPS, widely acknowledged to play a dominant role in biofilm structure.
properties. Christensen and Characklis (1990) even went so far as to say, with respect to
the importance of extracellular polymers to biofilm phenomena, that the presence of
extracellular polymers is responsible for the integrity of the biofilms.

With the time scale of microbial processes known, and after observing the
results of Series 0X – 23X, additional series were identified and run to examine biofilm
stress response under varying flow and material model coefficients over much longer
time periods. This was undertaken in the interest of identifying biofilm cluster behavior
which would result in long-term stability or long-term instability.

Investigation of Longer Time Scale

First and foremost, a characteristic behavior was identified to differentiate
between long-term stability and instability. Series 0X (Figure 16) demonstrated that the
deflection of the biofilm undergoes an inflection point, after which the deflection rate
begins to increase. The assumption was made that if this behavior is demonstrated before
some characteristic generation time, the deformation rate will continue to increase,
making microbial processes increasingly insignificant. Likewise, if this behavior was not
observed prior to some characteristic generation time, the assumption could be made that
microbial processes will influence the biofilm stability, leading to long-term viability.

Assuming a conservative characteristic generation time would mean choosing
one slightly shorter than those known for given microbial populations. Given the mixed-
culture nature of most naturally occurring biofilm colonies, it was decided to take a
characteristic time of the same order of magnitude as the shorter generation times given
in Table 5. Thus, a characteristic generation time of 0.1 hours was chosen. In light of methods of biofilm removal which utilize increased flow as a means of removal, assigning a shorter window of opportunity is to err on the conservative side.

Simulations were run which encompassed 1000 seconds (16 minutes, 40 seconds) and 3600 seconds (1 hour), both considering changes in Maxwell material parameters and variations in velocity. Table 6 shows simulation titles, the corresponding material parameter values, mean channel velocity and the duration of the simulation. Simulation numbers listed in Table 6 are preceded by an “L” to reflect the fact that a longer time was considered than in previous Series. The results of these simulations can be seen in Figures 31-33 below.
Table 6 – Long time duration parametric series. Parameter values are listed for each simulation as well as mean channel velocity and simulation duration. Values which were varied for any given Series are bold.

<table>
<thead>
<tr>
<th>Series</th>
<th>Channel Velocity</th>
<th>Duration</th>
<th>$G_1$</th>
<th>$\eta_1$</th>
<th>$\tau_1$</th>
<th>$G_2$</th>
<th>$\eta_2$</th>
<th>$\tau_2$</th>
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<tbody>
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<td>mm/s</td>
<td>s</td>
<td>kg/mm-s$^2$</td>
<td>kg/mm-s</td>
<td>s</td>
<td>kg/mm-s$^2$</td>
<td>kg/mm-s</td>
<td>s</td>
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<td>3600</td>
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<td>5</td>
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<td>150</td>
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<td>20</td>
<td>100</td>
<td>5</td>
</tr>
<tr>
<td>L022</td>
<td>500</td>
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</table>
Figure 31 – Series L02. Velocity was varied, material coefficients were held constant. Duration of simulation was 3600 seconds (1 hour). Only one simulation finished the 3600 second run. Other simulations terminated early due to excessive deformation.
Figure 32 – Series L03. Maxwell material coefficients were varied. Mean channel velocity was held constant at 1000 mm/s. Simulation duration was 1000 seconds (~16 minutes). Three simulations continued to completion.
Figure 33 – Series L04. Velocity was varied while holding material coefficients steady. Simulation duration was 1000 seconds (~16 minutes). Only two simulations resulted in excessive deformations.

It is clear most of the simulations were not able to continue to completion of the time duration specified. A closer look at the time range over which deformation behavior occurred indicates that most samples exhibited the transition from slowing deformation to accelerating deformation. Figure 34 below depicts the behavior of the biofilm cluster in Series L03 over a smaller time range, elucidating the inflection point.
Figure 34 – Series L03 with a shorter time span being considered. The shorter time scale elucidates the inflection point in some sets, demonstrating the transition to accelerating deformation.

Determining the position of the transition to accelerated deformation was accomplished by locating the inflection point. Taking the slope of the curve at data point $i$ to be:

$$S_i = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$  \hspace{1cm} (34)$$

In equation (34), $y$ corresponds to displacement and $x$ corresponds to time. Using this method, the slope was determined at each point. The expression in equation (34) is simply the numerical equivalent to a derivative. The point at which the slope was the
lowest (i.e. second derivative was zero) was taken as the inflection point. Use of data files created by ANSYS as specified in the ADPL made this procedure quite simple. In some cases, simulations did not ever reach a point of inflection suggesting that through the duration of the run deformation rates continued to decrease. The location of inflection points are indicated in Figures 35-37 below.

Figure 35 – Inflection points indicated for Series L02. Areas shaded represent biofilm behavior that is speculated to result in long-term colony stability. Transition to a time period over which microbial processes become significant is indicated. Set L021 maintained a decreasing rate of deformation, while Set L029 never showed a decreasing rate. Neither set ever exhibited an inflection point. Set L021b was run after Sets L021-L029 to “fill the gap” between L021 and L022.
Figure 36 – Series L03 with inflection point indicated. Areas shaded represent biofilm behavior that is speculated to result in long-term colony stability. Transition to a time period over which microbial processes become significant is indicated. Sets L038 and L039 maintained a decreasing rate of deformation, never exhibiting an inflection point.
Figure 37 – Series L04 with inflection points indicated. Areas shaded represent biofilm behavior that is speculated to result in long-term colony stability. Transition to a time period over which microbial processes become significant is indicated. Sets L041 through L045 maintained a decreasing rate of deformation, never exhibiting an inflection point. Note that the inflection point for Set L047 occurs before the transition indicating microbial processes become significant. In contrast, Set L046 experiences inflection well past the transition indicating that microbial processes become significant.

If biofilm is truly a viscoelastic fluid, the fact that biofilm persists in any environment where it is subjected to constant fluid induced forces such as water distribution pipes, or recirculating cooling systems, indicates a limitation in the Burger fluid model description. Even relatively small applied forces, when considered over long time periods, would serve to remove biofilm from any substratum to which it has attached if biofilm behaved, over long time periods, as a viscoelastic fluid.
In any simulation during which convergence was not achieved, some unique trends appeared. Namely, the transition from a decreasing rate of deformation to an increasing deformation rate was observed, indicated by an inflection point in the deformation curves, was observed. In a small number of cases, the same transition appeared even in simulations which converged through the duration. The effect of accelerated deformation due to the interplay between fluid induced forces and biofilm deformation may very well be the mechanism of large-scale detachment. If the transition to accelerated deformation rate takes place in a time period smaller than a characteristic generation time, it is likely that large-scale detachment is imminent.
DISCUSSION AND APPLICATION OF RESULTS

The results presented in the previous chapter can be used in a number of different ways to better understand biofilm behavior. Firstly, however, the mechanisms involved in the complex relationship between biofilm and its flowing environment should be considered, as well as the similarities between the model and previous experimental work.

Comparison to Experimental Work

One simple way to judge if the results of the simulations were reasonable was to compare the relative strain exhibited by the model to the strain observed in experimental work. Since the work done by Stoodley et al. (1999) was the basis for this work, it was chosen for comparison. While the biofilm observed by Stoodley et al. (1999) was clearly not a cube, a comparison of shear deformation angles is of value by showing consistency between the experimentally observed response and the computer model.

Using the information reported in the experimental work, an approximation of the shear angle of a biofilm cluster subjected to an increased fluid flow rate can be made. The shear angle is taken to be the angle through which the leading edge of the biofilm surface rotates as a result in changes in fluid flow rates. Stoodley et al. (1999) recorded the position of fluorescent latex particles stuck to the biofilm through image analysis to determine the angle of shear deformation. The angle of shear deformation shown by the investigation was estimated to be 11 degrees after being subjected to a fluid flow averaging 1000 mm/s.
Reported displacement of the biofilm cluster in the ANSYS model was used to determine the shear deformation angle. For Series 0X, shear angles ranged from 0.9 to 31 degrees. Since the displacement of the top planiform centroid of the biofilm was used in calculating the shear angle, the lower values of material model parameters resulted in greater final shear angles. Simulations which did not converge through the duration of the run reflected shear deformation angles of about 30 degrees. The range of values for the shear deformation angle matches the observed behavior in the experimental setup of Stoodley et al. (1999).

**Laminar Sublayer**

In all closed conduits, flowing fluid has at least a small region of laminar flow near the boundary. This region is considered the laminar sublayer in conduits exhibiting turbulent flow. Approximations for the thickness of this layer can be made based upon the fluid viscosity and the bulk flow rate (Cengel and Cimbala, 2006). In the case of the channel modeled with ANSYS, the laminar sublayer thickness is approximately equal to 0.025 mm when the average channel fluid velocity is 1000 mm/s. The biofilm height of 0.3 mm is significantly higher than the laminar sublayer thickness. Even in simulations with varying average channel velocities, the laminar sublayer remained small in comparison to the height of the biofilm. Further from the boundary, however, the flow is turbulent. The inertia of the flowing water dominates behavior in this turbulent region.

In simulations which exhibited significant deformations, it was assumed that the combination of lift and drag forces drew the biofilm further into the turbulent flow
region. The effect of the resulting increase in fluid forces led to further deformation. The combination of increasing lift and drag forces, due to the deformation of the biofilm, and the increasing deformation, due to the resulting increase in fluid forces acting on the biofilm, seem to have led to the behavior seen in Figures 35-37.

**Application of Model**

As discussed, the results showed a trend indicating that a transition to increasing deformation rate takes place in biofilm clusters subjected to fluid-induced forces. Additionally, it is proposed that a Burger fluid material model is limited in the time scale through which it is applicable. The model can be adjusted to mimic industrial settings if the flow rate and geometry of the system is known. Armed with such information, simulations which mimic the system conditions could be identified and run with varying material model parameters. Examination of the results of the simulations could be used to identify a range of possible material model parameter values based on the assumption that parameter values resulting in accelerated deformation over a short time scale would not reflect viable biofilm behavior. Information of this sort will allow system operators to identify conditions which are more likely to induce biofilm detachment.
SUMMARY

Biofilm is an omnipresent phenomenon that impacts many industries and professions. In the context of civil engineering, biofilm exists as a problem for clean and efficient water distribution methods. In the past, the manner in which biofilm interacts with flowing water has remained an area of study which has received limited investigation with respect to the mechanical material properties biofilm exhibits. More recently, however, investigators have paid closer attention to the mechanical properties of biofilm, resulting, in some cases, in complex constitutive relations through extensive mechanical testing procedures (Towler 2004, Sutton 2006). Additionally, the interactions between flowing water and biofilm have been observed in very clever ways, yielding results which corroborate the findings of mechanical testing procedures (Stoodley et al. 1999, 2002, Klapper 2002). This thesis presents a bridge between the mechanically measured constitutive relation and the observed in situ biofilm response to fluid induced forces through the development of a three dimensional numerical model. The project consisted of two stages: development of the numerical model utilizing the constitutive relation developed by Towler (2004), and application of the model through a parametric study which mimicked the experimental setup by Stoodley.

In the first stage, the material constitutive model was incorporated into a numerical model simulating a biofilm cluster attached to the interior wall of a fluid conduit. The model was developed using ANSYS. The model was scaled to match the test apparatus used by Stoodley et al. (1999, 2002). Once the model was developed, the second stage comprised the identification of a series of parametric simulations which
were run in order to elucidate some specific biofilm behavior. Deformation and drag forces were plotted to clarify the behavior of the biofilm. The results clearly showed the effects which material properties play in the dynamic interaction between water and biofilm.

Upon examining the results of the parametric studies, specific behavior was identified to be of importance when considering the likelihood of biofilm detachment. Specifically, a transition between slowing deformation and accelerating deformation took place for nearly all simulations run. Furthermore, indications pointed toward the fact that, given enough time, all simulations would have undergone the transition to accelerating deformation. The time over which microbial processes would influence biofilm material properties was established through identifying the generation time (the time it takes for a microbial species to undergo binary fission) for common biofilm species. If, during a simulation, the transition to accelerating deformation took place after to reaching the time determined to be significant for microbial activity to affect material properties, the assumption was made that the biofilm cluster would persist. Likewise, if the transition to accelerating deformation took place prior to the determined time, it was assumed that detachment was inevitable.

The model was used to demonstrate the response of a viscoelastic Burger fluid to forces induced by fluid flow around the biofilm. Empirical evidence suggests, by biofilm’s ubiquity, that over long time scales, biofilm does not act as a Burger fluid. Over short time scales, experimental results suggest that it does behave as a viscoelastic
Burger Fluid. For short time scales, the model which was developed can be used to identify the range of circumstances required to ensure detachment.

The model can surely be used for further investigations into the interaction between biofilm and flowing water. Matching the behavior of observed biofilm creep to the model, by varying material properties in the model, will allow the back-calculation of the biofilm properties through a non-destructive method. Further rheological testing of biofilm will certainly yield more confidence in the appropriate range of material properties. Additional work investigating the influence of growing conditions on biofilm strength will shed light on the range of biofilm material properties which can be expected in industrial settings. With the wide-ranging implications biofilm has on economics and health, the findings presented herein as well as the potential uses for the model are significant.
REFERENCES CITED


Center for Biofilm Engineering (CBE), Montana State University, Bozeman, Montana. Image © 1995, Peg Dirckx


Towler, B. 2005. Conversations regarding test procedures used and data collected during biofilm rheological tests.


APPENDIX A

ANSYS INPUT FOR BURGER FLUID FSI PROBLEM
Date: June, 2006

~Cube geometry
!
! SOLID185 used
!

Name Model

base_name = 'Cube'
number = '05'
!Define Jobname file string
m_job = STRCAT(base_name,'_')
m_job = STRCAT(m_job,number)
!Now, "job" is "Cube_05"
!
!Define this as the file name:
/filname, %m_job%, 1
!

Notes:
! This model simulates the 3-D reaction of a biofilm with varying material properties to varying flow-induced stress.
!
! Below is a schematic. Please keep in mind that the model is 3-D and, therefore, has 'depth'. Each of the three regions (A,B,C) are also three 'blocks' deep. Variables defined below (l_h,l_l,lc_h,tc_h,t_h,t_l) refer to the height (z-comp) of the respective locations. The first letter in the variable names refers to it's x-location, while the second refers to it's y-location, into the screen, where 'h' represents center heights, and 'l' represents the height at the x-z plane boundaries.
!
!
| Entrance . | X=1  | X=1c | X=1t | X=t | Exit |
| Region .   | X=1  | X=1c | X=1t | X=t | Region |
| ~           | ~    | ~    | ~    | ~    | ~    |
| \           | \    | \    | \    | \    | \    |
| /           | /    | /    | /    | /    | /    |
| Flow--->    | .    | .    | .    | .    | .    |
|             | A    | B    | C    | .    | .    |
|             | .    | .    | .    | .    | .    |
|             | ----x-----> | -> | b-typ | <- | <bx *and* gx---> | <------hx------> |
Steps in this FSI model

1.0 Model Parameters
  1.1 User Input
  1.2 Define Dependent Parameters
  1.3 Geometric User Inputs For Building Model
  1.4 Node Division Parameters

2.0 Fluid Analysis Setup.
  2.1 Fluid Keypoints
  2.2 Fluid Volumes
  2.3 Fluid Region Nodes
  2.4 Fluid Element Type Defined
  2.5 Fluid Types, Constants And Properties Defined
  2.6 Fluid Mesh Created
  2.7 Fluid Boundary Conditions
  2.8 Fluid Properties Defined
  2.9 Fluid Solution Controls

3.0 Structural Analysis Setup
  3.1 Structural Keypoints
  3.2 Structural Volumes
  3.3 Structural Nodes Defined
  3.4 Structural Element Type Defined
  3.5 Structural Properties Defined
  3.6 Structural Types, Constants, Properties Defined
  3.7 Structural Mesh Created
  3.8 Structural Boundary Conditions

4.0 Fluid-Structural Interaction
  4.1 Flag Fluid-Structural Interfaces
  4.2 Fluid-Structural Solution Options

5.0 Solution
  5.1 Define Monitor DOFs
  5.2 Labe Nodes for Observation
  5.3 Solve Model

6.0 Post Processing
  6.1 Set View
  6.2 Prony Series Parameter File
  6.3 Resultant Surface Force Calculation
  6.4 Stress at Certain Nodes
  6.5 Maximum Stress

End Of File

Units used in this model:

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<td>F/L^2</td>
<td>1 kg/m*s^2</td>
<td>10^-3 kg/mm*s^2</td>
<td>Pressure, Young's</td>
</tr>
</tbody>
</table>
/COM ...Step 1.0 - Model Parameters.................................

/COM ...Step 1.1 - User-Defined Parameters.........................

!User Input: Geometric Parameters
hc = 3 !Height of channel (mm)
w = 3 !Width of channel (mm)
l = 40 !Length of channel (mm)
hh = hc/2 !Half-height (mm)
hw = wc/2 !Half-width (mm)
hl = l/2 !Half-length (mm)
b = 0.1 !Size of blocks used in biofilm formation

!User Input: Fluid Parameters
vx = 1000.0 !Inlet X-dir velocity (mm/s)
v = 0.0 !Inlet Y-dir velocity (mm/s)
vz = 0.0 !Inlet Z-dir velocity (mm/s)
ro = 0.000001 !Density of water (kg/mm^3)
m = 0.000001 !Dynamic viscosity of water (kg/mm-s)

!User Input: Solid Parameters
G1 = 10 !Shear mod. for Max. (- -) spring(kg/mm-s^2)
h1 = 150 !Viscous coef. for Max. (- -) dashpot(kg/mm-s)
G2 = 20 !Shear mod. for Kelvin (||) spring(kg/mm-s^2)
h2 = 100 !Viscous coef. for Kelvin (||) dashpot(kg/mm-s)
PR = 0.33 !Poisson's Ratio for Biofilm
DE = 0.000001 !Mass Density of Biofilm (kg/mm^3)

!User Input: Controls
!Solution Control (c)
!Relaxation coefficients (r)
c_time = 30 !Total time of run (sec)
c_loadtime = 5 !Time to apply the FSI surface loads(sec)
c_dFSI = 0.25 !Time step FSI loop (Mult. of c_time)(sec)
c_dS = 0.25 !Time step for solid solution loop
!stagger iterations in FSI loop
!Global iterations for fluid solutions
!ON/OFF Switches
!SWITCH - Mesh-morphing switch. 0 = OFF, 1 = ON
!SWITCH - Solve? 0 = PREP only, 1 = SOLU
!SWITCH - Inlet vel. dist. 0 = uniform, 1 = Ven.
!ON/OFF Switch for Turbulence.
c_TURB = 1 ! SWITCH - Activate turb. eqns?. 0 = NO, 1 = YES
r_TM = 2 !Type of turbulence model (1-8, See FLDATA24)

!ON/OFF Switches for convergence techniques
!FLDATA,STAB,lab,value ! Stability controls
c_STABT = 0 ! SWITCH - applied to Turbulence
r_ST = 100000 ! defaults to 1.0*10^15
c_STABM = 0 ! SWITCH - applied to Momentum
r_SM = 100000 ! defaults to 1.0*10^15
c_STABP = 0 ! SWITCH - applied to Pressure
r_SP = 100000 ! defaults to 1.0*10^15
c_STABV = 0 ! SWITCH - applied to Viscosity
r_SV = 1 ! defaults to 0.0

!FLDATA,MIR,lab,value ! Modified Inertial Relaxation
c_MIRM = 0 ! SWITCH - Momentum. 0 = OFF, 1 = ON
r_MM = 0.5 ! defaults to 0.0
c_MIRT = 0 ! SWITCH - Turbulence. 0 = OFF, 1 = ON
r_MT = 0.5 ! defaults to 0.0

!FLDATA,RELX,lab,value ! Solution property relaxation factors
c_RELXX = 0 ! SWITCH - Relaxation of VX
r_RX = 1 ! defaults to 0.5
c_RELXY = 0 ! SWITCH - Relaxation of VY
r_RY = 1 ! defaults to 0.5
c_RELXZ = 0 ! SWITCH - Relaxation of VZ
r_RZ = 1 ! defaults to 0.5
c_RELXP = 0 ! SWITCH - Relaxation of PRES
r_RP = 1 ! defaults to 0.5
c_RELXE = 0 ! SWITCH - Relaxation of ENKE
r_RE = 1 ! defaults to 0.5
c_RELXEV = 0 ! SWITCH - Relaxation of EVIS (eff. Visc)
r_REV = 1 ! defaults to 0.5
c_RELXV = 0 ! SWITCH - Relaxation of VISC
r_RV = 1 ! defaults to 0.5

/COM ...Step 1.2 - Dependent Parameters.........................

Pi = 2*ASIN(1) ! Defines Pi

!Dependent Hydrodynamic Parameters
nu = mu/ro ! Kinematic viscosity (mm^2/s)
Re = vx*hc/nu ! Reynolds # of channel flow (-)
ff = (0.316/(Re)**0.25) ! Friction factor estimated (smooth walls)
!Relaxation modulus development.
!Intermediate parameters used in conversion to Prony Series \((i)\)

\[
i_p0 = 1
\]

\[
i_p1 = h1/G1+h1/G2+h2/G2
\]

\[
i_p2 = h1*h2/(G1*G2)
\]

\[
i_q1 = h1
\]

\[
i_q2 = h1*h2/G2
\]

\[
i_A = \left((i_p1)^2-(4*(i_p2))\right)^{(1/2)}
\]

\[
i_r1 = \frac{i_p1-i_A}{2*i_p2}
\]

\[
i_r2 = \frac{i_p1+i_A}{2*i_p2}
\]

\[
i_ginf = 0 \quad \text{! Constant for any Burger model}
\]

\[
i_g1 = \frac{i_q1-i_q2*i_r1}{i_A} \quad \text{! Equivalent 1st Maxwell shear coef}
\]

\[
i_g2 = -\frac{i_q1-i_q2*i_r2}{i_A} \quad \text{! Equivalent 2nd Maxwell shear coef}
\]

\[
i_g0 = i_ginf+i_g1+i_g2
\]

!Burger parameters represented by Prony series

\[
s_E0 = i_g0*2*(1+PR)
\]

\[
s_A1 = i_g1/i_g0
\]

\[
s_TAU1 = \frac{1}{i_r1} \quad \text{! Equiv 1st Maxwell relaxation time}
\]

\[
s_A2 = i_g2/i_g0
\]

\[
s_TAU2 = \frac{1}{i_r2} \quad \text{! Equiv 2nd Maxwell relaxation time}
\]

!Additional parameters used in generating the analytical solution

\[
s_E1 = i_g1*2*(1+PR) \quad \text{! Equiv 1st Maxwell elastic coeff.}
\]

\[
s_E2 = i_g2*2*(1+PR) \quad \text{! Equiv 2nd Maxwell elastic coeff.}
\]

ALLSEL,ALL
SAVE

/title, 3-D Biofilm FSI, RE=%Re%,G1=%G1%,h1=%h1%,G2=%G2%,h2=%h2%

/COM ... Step 1.3 - Geometric User Inputs for Building Model.....

!Define locations (x's, y's and z's) of regions

!DO NOT CHANGE VARIABLE BELOW! Except, and only if you know
!what you're doing:
!
! Denominator of 'bx' term (make it match that of 'gx')
! Values of "Biofilm Geometry (Z-locations)"
!
! More specifically:
!
\[
\text{l_h, l_l, lc_h, tc_h, t_h, and t_l}
\]

!X-locations.

ax=-1c/2 \quad \text{!Entrance (KP's=101+)}
bx=-1c/20 \quad \text{!End of entrance region (KP's=201+)}
 cx=-1.5*b \quad \text{!Leading face of biofilm (KP's=301+)}
ax=-0.5*b \quad \text{!Second set in biofilm (KP's=401+)}
ex=0.5*b \quad \text{!Third set in biofilm (KP's=501+)}
fx=1.5*b \quad \text{!Trailing edge of biofilm (KP's=601+)}
gx=1c/20 \quad \text{!Beginning of exit region (KP's=701+)}
hx=1c/2 \quad \text{!Exit (KP's=801+)}

bfrx=gx-bx !Biofilm region length in x-direction
x1=bx
x2=bx+(1*bfrx/(3))
x3=bx+(2*bfrx/(3))
x4=gx

!Y-locations.
ay=-wc/2 !Stream-right of channel
by=-1.5*b !Stream-right edge of biofilm
cy=-0.5*b !
dy=0.5*b !
ey=1.5*b !Stream-left edge of biofilm
fy=wc/2 !Stream-left of channel

bfry=ay-fy !Biofilm region width in y-direction.
y1=ay
y2=ay-(1*bfry/(3))
y3=ay-(2*bfry/(3))
y4=fy

!Z-locations.
az=0 !Channel base
bz=hc !Channel top

!Biofilm geometry (Z-locations)
l_h=0.3 !Leading edge_high (centers)
l_l=0.3 !Leading edge_low (edges)
lc_h=0.3 !Center_high
lc_l=lc_h-l_h+l_l !Center_low
tc_h=0.3 !Trailing center_high
t_h=0.3 !Trailing edge_high (centers)
t_l=0.3 !Trailing edge_low (edges)
tc_l=tc_h-t_h+l_l !Trailing center_low

z0=az
z1=bz

/COM ... Step 1.4 - Node Division Parameters.........................

!Define number of nodes on pertinent lines

bnx=2 !Number of divisions in biofilm pieces
bny=bnx
bnz=3*bnx
d_i=6 !Number of divisions along interior
!lines of biofilm region
!In entrance/exit region
d_{eh}=bnz !Number of nodal divs along ent/ex height
d_{ew}=3*bny !Number of nodal divs along ent/ex width
d_{el}=16 !Number of nodal divs along ent/ex length

!Bias of divisions towards biofilm in entrance/exit region.
be_n=0.5 !Nodal bias (Watch the sign!)

!Bias of divisions towards biofilm in "interior" lines
bi_n=0.2

ALLSEL, ALL
SAVE

/PREP7 !Enter Preprocessor

/COM ... Step 2.0 - Fluid Analysis Set-Up.........................

/COM ... Step 2.1 - Fluid Keypoints, etc............................

!Fluid Region Keypoints:

!Entrance Keypoints.
K,101,ax,ay,az
K,102,ax,fy,az
K,103,ax,fy,bz
K,104,ax,ay,bz

K,111,bx,ay,az
K,112,bx,fy,az
K,113,bx,fy,bz
K,114,bx,ay,bz

!Upstream Keypoints.
K,201,x1,y1,az
K,202,x1,y2,az
K,203,x1,y3,az
K,204,x1,y4,az
K,205,x1,y1,bz
K,206,x1,y2,bz
K,207,x1,y3,bz
K,208,x1,y4,bz

K,211,cx,by,az
K,212,cx,cy,az
K,213,cx,dy,az
K,214,cx,ey,az
K,215,cx,by,l_l
K,216,cx,cy,l_h
K,217,cx,dy,l_h
K,218,cx,ey,l_l
!Biofilm-1 Keypoints (Leading edge)

K, 301, x1, ay, az
K, 302, cx, by, az
K, 303, cx, by, l_l
K, 304, cx, cy, l_h
K, 305, cx, dy, l_h
K, 306, cx, ey, l_l
K, 307, cx, ey, az
K, 308, x1, fy, az
K, 309, x1, y1, bz
K, 310, x1, y2, bz
K, 311, x1, y3, bz
K, 312, x1, y4, bz
K, 321, x2, ay, az
K, 322, dx, by, az
K, 323, dx, by, lc_l
K, 324, dx, cy, lc_h
K, 325, dx, dy, lc_h
K, 326, dx, ey, lc_l
K, 327, dx, ey, az
K, 328, x2, fy, az
K, 329, x2, y1, bz
K, 330, x2, y2, bz
K, 331, x2, y3, bz
K, 332, x2, y4, bz

!Biofilm-2 Keypoints

K, 401, x2, ay, az
K, 402, dx, by, az
K, 403, dx, by, lc_l
K, 404, dx, cy, lc_h
K, 405, dx, dy, lc_h
K, 406, dx, ey, lc_l
K, 407, dx, ey, az
K, 408, x2, fy, az
K, 409, x2, y1, bz
K, 410, x2, y2, bz
K, 411, x2, y3, bz
K, 412, x2, y4, bz
K, 421, x3, ay, az
K, 422, ex, by, az
K, 423, ex, by, tc_l
K, 424, ex, cy, tc_h
K, 425, ex, dy, tc_h
K, 426, ex, ey, tc_l
K, 427, ex, ey, az
K, 428, x3, fy, az
K, 429, x3, y1, bz
K, 430, x3, y2, bz
K, 431, x3, y3, bz
K, 432, x3, y4, bz

!Biofilm-3 Keypoints
K, 501, x3, ay, az
K, 502, ex, by, az
K, 503, ex, by, tc_l
K, 504, ex, cy, tc_h
K, 505, ex, dy, tc_h
K, 506, ex, ey, tc_l
K, 507, ex, ey, az
K, 508, x3, fy, az
K, 509, x3, y1, bz
K, 510, x3, y2, bz
K, 511, x3, y3, bz
K, 512, x3, y4, bz

K, 521, x4, ay, az
K, 522, fx, by, az
K, 523, fx, by, l_l
K, 524, fx, cy, l_h
K, 525, fx, dy, l_h
K, 526, fx, ey, l_l
K, 527, fx, ey, az
K, 528, x4, fy, az
K, 529, x4, y1, bz
K, 530, x4, y2, bz
K, 531, x4, y3, bz
K, 532, x4, y4, bz

!Downstream Keypoints
K, 601, fx, by, az
K, 602, fx, cy, az
K, 603, fx, dy, az
K, 604, fx, ey, az
K, 605, fx, by, t_l
K, 606, fx, cy, t_h
K, 607, fx, dy, t_h
K, 608, fx, ey, t_l

K, 611, gx, y1, az
K, 612, gx, y2, az
K, 613, gx, y3, az
K, 614, gx, y4, az
K, 615, x4, y1, bz
K, 616, x4, y2, bz
K, 617, x4, y3, bz
K, 618, x4, y4, bz

!Exit Keypoints.
K, 701, gx, ay, az
K, 702, gx, fy, az
K,703,gx, fy, bz
K,704,gx, ay, bz
K,711,hx, ay, az
K,712,hx, fy, az
K,713,hx, fy, bz
K,714,hx, ay, bz

!/COM ... Step 2.2 - Fluid Volumes.................................

!Entrance Region
!Set beginning numerical values assigned to KP's, lines, areas, 
!and volumes to 101
NUMSTR,KP,101  !New KP's will start at the # 101
NUMSTR,LINE,101  !Same for Lines
NUMSTR,AREA,101  !Same for Areas
NUMSTR,VOLU,101  !Same for Volumes
V,101,102,103,104,111,112,113,114

!Upstream region.
NUMSTR,KP,201  !New KP's will start at the # 201
NUMSTR,LINE,201  !Same for Lines
NUMSTR,AREA,201  !Same for Areas
NUMSTR,VOLU,201  !Same for Volumes
A,211,212,216,215  !Area 201
A,212,213,217,216  !Area 202
A,213,214,218,217  !Area 203
V,201,202,206,205,211,212,216,215
V,202,203,207,206,212,213,217,216
V,203,204,208,207,213,214,218,217

!Fluid Biofilm region-300
NUMSTR,KP,301  !New KP's will start at the # 301
NUMSTR,LINE,301  !Same for Lines
NUMSTR,AREA,301  !Same for Areas
NUMSTR,VOLU,301  !Same for Volumes
A,302,303,323,322  !Area 301
A,303,304,324,323  !Area 302
A,304,305,325,324  !Area 303
A,305,306,326,325  !Area 304
V,301,302,303,309,321,322,323,329
V,303,304,310,309,323,324,330,329
V,304,305,311,310,324,325,331,330
V,305,306,312,311,325,326,332,331
V,307,308,312,306,327,328,332,326
!Fluid Biofilm region-400
NUMSTR,KP,401  !New KP's will start at the # 401
NUMSTR,LINE,401  !Same for Lines
NUMSTR,AREA,401  !Same for Areas
NUMSTR,VOLU,401  !Same for Volumes
A,402,403,423,422 !Area 401
A,403,404,424,423 !Area 402
A,404,405,425,424 !Area 403
A,405,406,426,425 !Area 404
A,406,407,427,426 !Area 405
V,401,402,403,409,421,422,423,429
V,403,404,410,409,423,424,430,429
V,404,405,411,410,424,425,431,430
V,405,406,412,411,425,426,432,431
V,407,408,412,406,427,428,432,426

!Fluid Biofilm region-500
NUMSTR,KP,501  !New KP's will start at the # 501
NUMSTR,LINE,501  !Same for Lines
NUMSTR,AREA,501  !Same for Areas
NUMSTR,VOLU,501  !Same for Volumes
A,502,503,523,522 !Area 501
A,503,504,524,523 !Area 502
A,504,505,525,524 !Area 503
A,505,506,526,525 !Area 504
A,506,507,527,526 !Area 505
V,501,502,503,509,521,522,523,529
V,503,504,510,509,523,524,530,529
V,504,505,511,510,524,525,531,530
V,505,506,512,511,525,526,532,531
V,507,508,512,506,527,528,532,526

!Downstream region.
NUMSTR,KP,601  !New KP's will start at the # 601
NUMSTR,LINE,601  !Same for Lines
NUMSTR,AREA,601  !Same for Areas
NUMSTR,VOLU,601  !Same for Volumes
A,611,612,616,615 !Area 601
A,612,613,617,616 !Area 602
A,613,614,618,617 !Area 603
V,601,602,606,605,611,612,616,615
V,602,603,607,606,612,613,617,616
V,603,604,608,607,613,614,618,617

!Exit region
NUMSTR,KP,701  !New KP's will start at the # 701
NUMSTR,LINE,701  !Same for Lines
NUMSTR,AREA,701  !Same for Areas
NUMSTR,VOLU,701

V,701,702,703,704,711,712,713,714

/COM ... Step 2.3 - Fluid Region Nodes

!Create nodes on fluid volume lines.

NUMSTR,NODE,10001
NUMSTR,ELEM,10001

!Entrance Region

LSEL,S,,,101,103,2
LSEL,A,,,106,110,4
LESIZE,ALL,,,d_ew
LSEL,S,,,102,104,2
LSEL,A,,,108,112,4
LESIZE,ALL,,,d_eh

LSEL,S,,,105
LESIZE,ALL,,,d_el,be_n
LSEL,S,,,107,111,2
LESIZE,ALL,,,d_el,1/be_n

!Upstream region

!Interior lines
LSEL,S,,,215
LSEL,A,,,222
LSEL,A,,,227
LESIZE,ALL,,,d_i,bi_n
LSEL,S,,,216,218,1
LSEL,A,,,223
LSEL,A,,,228
LESIZE,ALL,,,d_i,1/bi_n

!Y-lines
LSEL,S,,,201,207,2
LSEL,A,,,208,210,2
LSEL,A,,,211,213,2
LSEL,A,,,219,221,2
LSEL,A,,,224,226,2
LESIZE,ALL,,,bny

!Z-lines
LSEL,S,,,202,206,2
LSEL,A,,,209,212,3
LSEL,A,,,214,220,6
LSEL,A,,,225
LESIZE,ALL,,,bnz

!Biofilm region

!Interior lines
LSEL,S,,,317
LSEL, A,,, 343
LESIZE, ALL,,, d_i, bi_n
LSEL, S,,, 318
LSEL, A,,, 320
LSEL, A,,, 322
LSEL, A,,, 325
LSEL, A,,, 327
LSEL, A,,, 330
LSEL, A,,, 332
LSEL, A,,, 335
LSEL, A,,, 337
LSEL, A,,, 340
LESIZE, ALL,,, d_i, 1/bi_n

!X-lines
LSEL, S,,, 302
LSEL, A,,, 304
LSEL, A,,, 306
LSEL, A,,, 309
LSEL, A,,, 312
LSEL, A,,, 315
LSEL, A,,, 321
LSEL, A,,, 323
LSEL, A,,, 328
LSEL, A,,, 333
LSEL, A,,, 338
LSEL, A,,, 342
LESIZE, ALL,,, bnx

!Y-lines
LSEL, S,,, 305
LSEL, A,,, 307
LSEL, A,,, 308
LSEL, A,,, 310
LSEL, A,,, 311
LSEL, A,,, 313
LSEL, A,,, 326
LSEL, A,,, 329
LSEL, A,,, 331
LSEL, A,,, 334
LSEL, A,,, 336
LSEL, A,,, 339
LESIZE, ALL,,, bny

!Z lines
LSEL, S,,, 301
LSEL, A,,, 303
LSEL, A,,, 314
LSEL, A,,, 316
LSEL, A,,, 319
LSEL, A,,, 324
LSEL, A,,, 341
LSEL, A,,, 344
LESIZE, ALL,,, bnz
!Second region
!Interior lines
LSEL,S,,,417
LSEL,A,,,443
LESIZE,ALL,,,d_i,bi_n
LSEL,S,,,418
LSEL,A,,,420
LSEL,A,,,422
LSEL,A,,,425
LSEL,A,,,427
LSEL,A,,,430
LSEL,A,,,432
LSEL,A,,,435
LSEL,A,,,437
LSEL,A,,,440
LESIZE,ALL,,,d_i,1/bi_n

!X–lines
LSEL,S,,,402
LSEL,A,,,404
LSEL,A,,,406
LSEL,A,,,409
LSEL,A,,,412
LSEL,A,,,415
LSEL,A,,,421
LSEL,A,,,423
LSEL,A,,,428
LSEL,A,,,433
LSEL,A,,,438
LSEL,A,,,442
LESIZE,ALL,,,bnx

!Y–lines
LSEL,S,,,405
LSEL,A,,,407
LSEL,A,,,408
LSEL,A,,,410
LSEL,A,,,411
LSEL,A,,,413
LSEL,A,,,426
LSEL,A,,,429
LSEL,A,,,431
LSEL,A,,,434
LSEL,A,,,436
LSEL,A,,,439
LESIZE,ALL,,,bny

!Z lines
LSEL,S,,,401
LSEL,A,,,403
LSEL,A,,,414
LSEL,A,,,416
LSEL,A,,,419
LSEL,A,,,424
LSEL,A,,,441
LSEL,A,,,444
LESIZE,ALL,,,bnz

!Third region!Interior lines
LSEL,S,,,517
LSEL,A,,,543
LESIZE,ALL,,,d_i,bi_n
LSEL,A,,,518
LSEL,A,,,520
LSEL,A,,,522
LSEL,A,,,525
LSEL,A,,,527
LSEL,A,,,530
LSEL,A,,,532
LSEL,A,,,535
LSEL,A,,,537
LSEL,A,,,540
LESIZE,ALL,,,d_i,1/bi_n

!X-lines
LSEL,S,,,502
LSEL,A,,,504
LSEL,A,,,506
LSEL,A,,,509
LSEL,A,,,512
LSEL,A,,,515
LSEL,A,,,521
LSEL,A,,,523
LSEL,A,,,528
LSEL,A,,,533
LSEL,A,,,538
LSEL,A,,,542
LESIZE,ALL,,,bnx

!Y-lines
LSEL,S,,,505
LSEL,A,,,507
LSEL,A,,,508
LSEL,A,,,510
LSEL,A,,,511
LSEL,A,,,513
LSEL,A,,,526
LSEL,A,,,529
LSEL,A,,,531
LSEL,A,,,534
LSEL,A,,,536
LSEL,A,,,539
LESIZE,ALL,,,bny

!Z lines
LSEL,S,,,501
LSEL,A,,,503
LSEL,A,,,514
LSEL,A,,,516
LSEL,A,,,519
LSEL,A,,,524
LSEL,A,,,541
LSEL,A,,,544
LESIZE,ALL,,,bnz

!Downstream Region*******************
!Interior lines
LSEL,S,,,616
LSEL,A,,,617
LSEL,A,,,618
LSEL,A,,,623
LSEL,A,,,628
LESIZE,ALL,,,d_i,bi_n
LSEL,S,,,615
LSEL,A,,,627
LSEL,A,,,622
LESIZE,ALL,,,d_i,1/bi_n

!Y-lines
LSEL,S,,,601,607,2
LSEL,A,,,608,610,2
LSEL,A,,,611,613,2
LSEL,A,,,619,621,2
LSEL,A,,,624,626,2
LESIZE,ALL,,,bny

!Z-lines
LSEL,S,,,602,606,2
LSEL,A,,,609,612,3
LSEL,A,,,614,620,6
LSEL,A,,,625
LESIZE,ALL,,,bnz

!Exit Region********************************
LSEL,S,,,701,703,2 !Select upstream entrance lines
LSEL,A,,,706,710,4 !Select downstream entrance lines
LESIZE,ALL,,,d_ew
LSEL,S,,,702,704,2
LSEL,A,,,708,712,4
LESIZE,ALL,,,d_eh

LSEL,S,,,707,711,2 !Channel length lines in entrance region
LESIZE,ALL,,,d_el,be_n
LSEL,S,,,705
LESIZE,ALL,,,d_el,1/be_n

ALLSEL,ALL
SAVE
/COM ... Step 2.4 - Fluid Element Type Defined....................

ET,1,FLUID142 !Element Type 1 is Fluid 142 (3-D)
*IF,c_ALE,EQ,1,THEN
  KEYOPT,1,4,1 ! Include if ALE meshing is turned
*ENDIF ! on w/FLDA,SOLU,ALE,TRUE command

/COM ... Step 2.5 - Fluid Type, Constants and Properties Defined.

TYPE,1 ! Enable Element Type 1
! No material or real constants are defined for fluid analysis.
! Fluid properties are defined with the FLDATA command below.

/COM ... Step 2.6 - Mesh Fluid Volumes.........................

!Specify mesh parameters for:
VSEL,S,,,100,800,1 !Select Fluid Volumes (The Channel)
MSHAPE,0,3D !Mesh with hexahedrons in 3-D
MSHKEY,1 !Use mapped meshing
VMESH,ALL !Mesh Fluid Volumes (Channel)

NUMMRG, NODE
NUMMRG, KP

ALLSEL, ALL
SAVE

/COM ... Step 2.7 - Fluid Boundary Conditions...................

!Gravity force simulated through application of positive accel.
g=9810 !Gravitational acceleration: mm/s^2
!ACEL,0,0,g !ACEL,X(#),Y(#),Z(#) !Entrance area (Area 101) given uniform velocity (X-dir)
ASEL,S,,,101
NSLA,S,1

D,ALL,VX,vx !Velocities vx, vy, vz defined above
D,ALL,VY,vy
D,ALL,VZ,vz

D,ALL,UX,0 !Entrance wall is made stationary
D,ALL,UY,0
D,ALL,UZ,0
!No-slip condition applied to channel wall boundaries

ASEL,S,,,102,105,1  !Select wall areas

ASEL,A,,,205
ASEL,A,,,210
ASEL,A,,,214

ASEL,A,,,307,309,2
ASEL,A,,,313,325,4
ASEL,A,,,324

ASEL,A,,,407,409,2
ASEL,A,,,413,425,4
ASEL,A,,,424

ASEL,A,,,507,509,2
ASEL,A,,,513,525,4
ASEL,A,,,524

ASEL,A,,,605
ASEL,A,,,610
ASEL,A,,,614

ASEL,A,,,702,705,1

NSLA,S,1

D,ALL,VX,0  !Set boundary velocity to zero
D,ALL,VY,0  !for all wall surfaces
D,ALL,VZ,0

D,ALL,UX,0  !Wall surfaces are stationary.
D,ALL,UY,0
D,ALL,UZ,0

!Exit pressure defined

ASEL,S,,,706  !Select exit surface
NSLA,S,1

D,ALL,PRES,0,1  !Assign a zero pressure at the exit area.

D,ALL,UX,0  !Exit wall is made stationary
D,ALL,UY,0
D,ALL,UZ,0

!Apply no-slip condition to the Fluid-biofilm interface

!Fluid realm surfaces

ASEL,S,,,201,203,1
ASEL,A,,,301,305,1
ASEL,A,,,401,405,1
ASEL,A,,,501,505,1
ASEL,A,,,604
ASEL,A,,,609
ASEL,A,,,613

NSLA,S,1

! All biofilm surface areas have been selected, now apply
! Boundary conditions to them.

D,ALL,VX,0
D,ALL,VY,0
D,ALL,VZ,0

/COM ... Step 2.8 - Fluid Properties Defined.....................

FLDATA,PROT,DENS,CONSTANT ! fluid density is constant
FLDATA,PROT,VISC,CONSTANT ! fluid viscosity is constant
FLDATA,NOMI,DENS,ro ! fluid density specified by 'ro'
FLDATA,NOMI,VISC,mu ! fluid viscosity specified by 'nu'

ALLSEL,ALL
SAVE

/COM ... Step 2.9 - Fluid Solution Control........................

FLDA,OUTP,TAUW,TRUE
FLDA,OUTP,YPLU,TRUE

! Fluid convergence criteria
FLDATA,TERM,VX,0.001 ! Conv. on VX term (0.01 default)

! Maximum number of iterations
! FLDATA,ITER,EXEC,c_iF ! # of fluid solution iterations
! (static)
FLDATA,TIME,GLOB,c_iF ! # of fluid solution iterations
! (transient)

! Output Frequency
FSOU,ALL ! Write each iteration

! Relaxation Value
FSRE,ALL,0.6 ! Set relaxation value

ALLSEL,ALL
SAVE

! Turbulence Settings
*IF,c_TURB,EQ,1,THEN
    FLDATA,SOLU,TURB,TRUE ! Turns on the turbulence model.
    FLDATA,TURB,MODL,r_TM ! Sets the turbulence model
*ENDIF
! Relaxation settings.
! Momentum relaxation.
*IF, c_MIRM, EQ, 1, THEN
   FLDATA, MIR, MOME, r_MM ! Sets momentum relaxation.
*ENDIF

! Turbulence relaxation.
*IF, c_MIRT, EQ, 1, THEN
   FLDATA, MIR, TURB, r_MT ! Sets turbulence relaxation.
*ENDIF

! Stability controls
! Stability control - Turbulence.
*IF, c_STABT, EQ, 1, THEN
   FLDATA, STAB, TURB, r_ST ! Sets turbulence stability.
*ENDIF

! Stability Control - Momentum
*IF, c_STABM, EQ, 1, THEN
   FLDATA, STAB, MOME, r_SM ! Sets momentum stability.
*ENDIF

! Stability Control - Pressure
*IF, c_STABP, EQ, 1, THEN
   FLDATA, STAB, PRES, r_SP ! Sets pressure stability.
*ENDIF

! Stability Control - Viscosity
*IF, c_STABV, EQ, 1, THEN
   FLDATA, STAB, VISC, r_SV ! Sets viscosity stability.
*ENDIF

! Relaxation controls
! Relaxation - Velocity - X
*IF, c_RELXX, EQ, 1, THEN
   FLDATA, RELX, VX, r_RX ! Sets VX relaxation.
*ENDIF

! Relaxation - Velocity - Y
*IF, c_RELXY, EQ, 1, THEN
   FLDATA, RELX, VY, r_RY ! Sets VY relaxation.
*ENDIF

! Relaxation - Velocity - Z
*IF, c_RELXZ, EQ, 1, THEN
   FLDATA, RELX, VZ, r_RZ ! Sets VZ relaxation.
*ENDIF

! Relaxation - Pressure
*IF, c_RELXP, EQ, 1, THEN
   FLDATA, RELX, PRES, r_RP ! Sets Pressure relaxation.
*ENDIF
!Relaxation - Kinetic Energy
*IF, c_RELXE, EQ, 1, THEN
   FLDATA, RELX, ENKE, r_RE ! Sets Kinetic Energy relaxation.
*ENDIF

!Relaxation - Effective Viscosity
*IF, c_RELXEV, EQ, 1, THEN
   FLDATA, RELX, EVIS, r_REV ! Sets effective visc. relaxation.
*ENDIF

!Relaxation - Viscosity
*IF, c_RELXV, EQ, 1, THEN
   FLDATA, RELX, VISC, r_RV ! Sets Viscosity relaxation.
*ENDIF

! general fluid solution options/controls
FLDATA, SOLU, TRAN, TRUE ! fluid solution is transient
FLDATA, ALGR, SEGR, SIMPLEN ! enhanced SIMPLEN sol. algorithm
*IF, c_ALE, EQ, 1, THEN
   FLDA, SOLU, ALE, TRUE ! activates ALE mesh-morphing
*ENDIF

! Pressure and momentum equation settings
FLDATA, SOLU, FLOW, TRUE ! solves pressure and momentum eqs.
FLDATA, ADVM, MOME, SUPG ! Use streamline upward
                        ! discretization on momentum eqn.
*IF, c_ALE, EQ, 1, THEN
   FLDATA, QUAD, MOMD, 2 ! Accuracy of quadrature
   FLDATA, QUAD, MOMA, 2 ! increased for ALE
   FLDATA, QUAD, MOMS, 2
   FLDATA, QUAD, PRSD, 2
   FLDATA, QUAD, PRSS, 2
*ENDIF

ALLSEL, ALL
SAVE

/COM ... Step 3.0 - Structural Analysis Setup.......................

/COM ... Step 3.1 - Structural Keypoints.........................

!Set beginning numerical values assigned to lines, areas, 
! and volumes to 1001
NUMSTR, LINE, 1001 !Same for Lines
NUMSTR, AREA, 1001 !Same for Areas
NUMSTR, VOLU, 1001 !Same for Volumes

K, 1301, cx, ay, az
K, 1302, cx, by, az
K, 1303, cx, cy, az
K, 1304, cx, dy, az
K, 1305, cx, ey, az
K,1306,cx,fy,az
K,1307,cx,ay,1_l
K,1308,cx,by,1_l
K,1309,cx,cy,1_h
K,1310,cx,dy,1_h
K,1311,cx,ey,1_l
K,1312,cx,fy,1_l

K,1321,dx,ay,az
K,1322,dx,by,az
K,1323,dx,cy,az
K,1324,dx,dy,az
K,1325,dx,ey,az
K,1326,dx,fy,az
K,1327,dx,ay,lc_l
K,1328,dx,by,lc_l
K,1329,dx,cy,lc_h
K,1330,dx,dy,lc_h
K,1331,dx,ey,lc_l
K,1332,dx,fy,lc_l

!Biofilm-2 Keypoints
K,1401,dx,ay,az
K,1402,dx,by,az
K,1403,dx,cy,az
K,1404,dx,dy,az
K,1405,dx,ey,az
K,1406,dx,fy,az
K,1407,dx,ay,lc_l
K,1408,dx,by,lc_l
K,1409,dx,cy,lc_h
K,1410,dx,dy,lc_h
K,1411,dx,ey,lc_l
K,1412,dx,fy,lc_l

K,1421,ex,ay,az
K,1422,ex,by,az
K,1423,ex,cy,az
K,1424,ex,dy,az
K,1425,ex,ey,az
K,1426,ex,fy,az
K,1427,ex,ay,tc_l
K,1428,ex,by,tc_l
K,1429,ex,cy,tc_h
K,1430,ex,dy,tc_h
K,1431,ex,ey,tc_l
K,1432,ex,fy,tc_l

!Biofilm-3 Keypoints
K,1501,ex,ay,az
K,1502,ex,by,az
K,1503,ex,cy,az
K,1504,ex,dy,az
K,1505,ex,ey,az
K,1506,ex,fy,az
K,1507,ex,ay,tc_l
K,1508,ex,by,tc_l
K,1509,ex,cy,tc_h
K,1510,ex,dy,tc_h
K,1511,ex,ey,tc_l
K,1512,ex,fy,tc_l

K,1521,fx,ay,az
K,1522,fx,by,az
K,1523,fx,cy,az
K,1524,fx,dy,az
K,1525,fx,ey,az
K,1526,fx,fy,az
K,1527,fx,ay,l_l
K,1528,fx,by,l_l
K,1529,fx,cy,l_h
K,1530,fx,dy,l_h
K,1531,fx,ey,l_l
K,1532,fx,fy,l_l

base=1300
L,base+02,base+03
L,base+03,base+04
L,base+04,base+05
L,base+02,base+08
L,base+03,base+09
L,base+04,base+10
L,base+05,base+11
L,base+08,base+09
L,base+09,base+10
L,base+10,base+11
L,base+02,base+22
L,base+03,base+23
L,base+04,base+24
L,base+05,base+25
L,base+08,base+28
L,base+09,base+29
L,base+10,base+30
L,base+11,base+31
L,base+22,base+23
L,base+23,base+24
L,base+24,base+25
L,base+22,base+28
L,base+23,base+29
L,base+24,base+30
L,base+25,base+31
L,base+28,base+29
L,base+29,base+30
L,base+30,base+31
NUMSTR, LINE, 2001

base=1400
L, base+02, base+03
L, base+03, base+04
L, base+04, base+05
L, base+02, base+08
L, base+03, base+09
L, base+04, base+10
L, base+05, base+11
L, base+08, base+09
L, base+09, base+10
L, base+10, base+11
L, base+02, base+22
L, base+03, base+23
L, base+04, base+24
L, base+05, base+25
L, base+08, base+28
L, base+09, base+29
L, base+10, base+30
L, base+11, base+31
L, base+22, base+23
L, base+23, base+24
L, base+24, base+25
L, base+22, base+28
L, base+23, base+29
L, base+24, base+30
L, base+25, base+31
L, base+28, base+29
L, base+29, base+30
L, base+30, base+31

NUMSTR, LINE, 3001

base=1500
L, base+02, base+03
L, base+03, base+04
L, base+04, base+05
L, base+02, base+08
L, base+03, base+09
L, base+04, base+10
L, base+05, base+11
L, base+08, base+09
L, base+09, base+10
L, base+10, base+11
L, base+02, base+22
L, base+03, base+23
L, base+04, base+24
L, base+05, base+25
L, base+08, base+28
L, base+09, base+29
L, base+10, base+30
L, base+11, base+31
L, base+22, base+23
L, base+23, base+24
L, base+24, base+25
L, base+22, base+28
L, base+23, base+29
L, base+24, base+30
L, base+25, base+31
L, base+28, base+29
L, base+29, base+30
L, base+30, base+31

/COM ... Step 3.2 - Structural Areas and Volumes.................

base=1300
A, base+2, base+3, base+9, base+8
A, base+3, base+4, base+10, base+9
A, base+4, base+5, base+11, base+10
A, base+2, base+8, base+28, base+22
A, base+8, base+9, base+29, base+28
A, base+9, base+10, base+30, base+29
A, base+10, base+11, base+31, base+30
A, base+11, base+05, base+25, base+31

base=1400
A, base+2, base+08, base+28, base+22
A, base+08, base+09, base+29, base+28
A, base+09, base+10, base+30, base+29
A, base+10, base+11, base+31, base+30
A, base+11, base+05, base+25, base+31

base=1500
A, base+2, base+8, base+28, base+22
A, base+8, base+9, base+29, base+28
A, base+9, base+10, base+30, base+29
A, base+10, base+11, base+31, base+30
A, base+11, base+05, base+25, base+31

A, base+22, base+23, base+29, base+28
A, base+23, base+24, base+30, base+29
A, base+24, base+25, base+31, base+30

Biofilm-1 Volume

base=1300
V, base+02, base+03, base+09, base+08, base+22, base+23, base+29, base+28
V, base+03, base+04, base+10, base+09, base+23, base+24, base+30, base+29
V, base+04, base+05, base+11, base+10, base+24, base+25, base+31, base+30

Biofilm-2 Volume

base=1400
V, base+02, base+03, base+09, base+08, base+22, base+23, base+29, base+28
V, base+03, base+04, base+10, base+09, base+23, base+24, base+30, base+29
V, base+04, base+05, base+11, base+10, base+24, base+25, base+31, base+30
!Biofilm-3 Volume
base=1500
V,base+02,base+03,base+09,base+08,base+22,base+23,base+29,base+28
V,base+03,base+04,base+10,base+09,base+23,base+24,base+30,base+29
V,base+04,base+05,base+11,base+10,base+24,base+25,base+31,base+30

VSEL,S,,,1000,2000
VGLUE,ALL

ALLSEL,ALL
SAVE

/COM ... Step 3.3 - Structural Nodes.................................

!Select Lines associated with biofilm structure
LSEL,S,,,1011,1018,1 !Select all x-direction lines.
LSEL,A,,,3037,3044,1
LSEL,A,,,3029,3036,1
LESIZE,ALL,,,bnx !Divide each line into [bnx] pieces

LSEL,S,,,1001,1003,1
LSEL,A,,,1008,1010,1
LSEL,A,,,1019,1021,1
LSEL,A,,,1026,1028,1
LSEL,A,,,2019,2021,1
LSEL,A,,,2026,2028,1
LSEL,A,,,3019,3021,1
LSEL,A,,,3026,3028,1

LESIZE,ALL,,,bny

LSEL,S,,,1004,1007,1
LSEL,A,,,1022,1025,1
LSEL,A,,,2022,2025,1
LSEL,A,,,3022,3025,1

LESIZE,ALL,,,bnz

/COM ... Step 3.4 - Structural Element Type Defined..............

!Format for defining Element Type:
!ET,ITYPE,Ename,KOP1,KOP2,KOP3,KOP4,KOP5,KOP6,INOPR

ET,2,SOLID185,,3 !Element Type 2 is Structural Solid 185(3-D)
!Keyopt (2),"2" indicates
!enhanced strain formulation
!"3" indicates simplified enhanced strain
/COM ... Step 3.5 - Set Biofilm Material Properties..............

MP,EX,2,s_E0 !Youngs Modulus (Material 2)
MP,PRXY,2,PR !Poisson's Ratio, Major (Material 2)
MP,DENS,2,DE !Mass Density
TB,PRONY,2,,2,SHEAR !Creates a Table of Prony Coefficients
   !Fills in the values of the Coefficients
TBDATA,1,s_A1,s_TAU1,s_A2,s_TAU2

/COM ... Step 3.6 - Enable Structural Types, Constants, Properties

TYPE,2 !Enable Element Type 2
REAL,2 !Enable Real Constants 2
MAT,2 !Enable Material 2

/COM ... Step 3.7 - Mesh Solid.............................

NUMSTR,LINE,1001 !Same for Lines
NUMSTR,AREA,1001 !Same for Areas
NUMSTR,VOLU,1001 !Same for Volumes
NUMSTR,NODE,1 !Numbering of nodes will begin at 1
NUMSTR,ELEM,1 !Numbering of Elements will begin at 1

!Specify mesh parameters for:
VSEL,S,,,1000,2000,1 !Select Solid Volumes (Biofilm)

MSHAPE,0,3D !Mesh using hexahedrons in 3-D
MSHKEY,1 !Use mapped meshing
VMESH,ALL !Mesh Solid Volumes (Biofilm Blob)

ALLSEL,ALL
SAVE

/COM ... Step 3.8 - Structural Boundary Conditions...............

ASEL,S,,,1022 !Selects areas defining base of biofilm
ASEL,A,,,1025
ASEL,A,,,1028
ASEL,A,,,1059
ASEL,A,,,1063
ASEL,A,,,1066
ASEL,A,,,1049
ASEL,A,,,1053
ASEL,A,,,1056

NSLA,S,1

D,ALL,UX,0 !Biofilm attachment surface is stationary
D,ALL,UY,0
D,ALL,UZ,0

ALLSEL,ALL
SAVE

/COM ... Step 4.0 - Fluid-Structural Interaction.................

/COM ... Step 4.1 - Flag Fluid-Structural Interfaces..............

! The SF command used below flags the fluid side of the biofilm boundary

! Select each area of the biofilm boundary (and the associated nodes) and specify that it is loaded surface in the FSI solution

ASEL,S,,,1001 ! Select areas ____
ASEL,A,,,1002
ASEL,A,,,1003
ASEL,A,,,1004
ASEL,A,,,1005
ASEL,A,,,1006
ASEL,A,,,1007
ASEL,A,,,1008
ASEL,A,,,1060
ASEL,A,,,1062
ASEL,A,,,1065
ASEL,A,,,1068
ASEL,A,,,1067
ASEL,A,,,1050
ASEL,A,,,1052
ASEL,A,,,1054
ASEL,A,,,1057
ASEL,A,,,1058
ASEL,A,,,1019
ASEL,A,,,1020
ASEL,A,,,1021
NSLA,S,1 ! Select nodes associated with that area
SF,ALL,FSIN,1 ! Flag as FSI load surface, labeled #____

! Now flag the areas associated with the Fluid

ASEL,S,,,201,203,1 ! Select areas ____
ASEL,A,,,301,305,1
ASEL,A,,,401,405,1
ASEL,A,,,501,505,1
ASEL,A,,,604
ASEL,A,,,609
ASEL,A,,,613
NSLA,S,1 ! Select nodes associated with that area
SF,ALL,FSIN,1 ! Flag as FSI load surface, labeled #____

ALLSEL,ALL
SAVE
Step 4.2 - Fluid Structure Interaction Solution Options.

NCNV,0,c_MAX

FSAN,ON !Turn on FSI analysis
FSOR,FLUID,SOLID !Solution order: Fluid, then Solid
FSTR,FLUID,TRAN !Fluid solution is transient
FSTR,SOLID,TRAN !Solid Solution is transient
FSIN,CONS !Interface load transfer is conservative

FLDA,OUTP,TAUW,TRUE
FLDA,OUTP,YPLU,TRUE

FSTI,c_time,c_loadtime !End time, Load time for FSI analysis
FSDT,c_dtFSI !Time step increment for FSI analysis
DELTIM,c_dtS,,,OFF !Time step increment for solid analysis
FLDATA,TIME,STEP,c_dtF !Time step increment for Fluid analysis

!Fluid convergence criteria
FLDATA,TERM,VX,0.001 !Conv. on VX term (0.01 default)

!Maximum number of iterations
!FLDATA,ITER,EXEC,c_iF !Number of fluid sol. iterations (static)
FLDATA,TIME,GLOBAL,c_iF !Number of fluid sol. iterations (trans)
FSIT,c_iFSI !FSI stagger iterations

!FSI convergence values
FSCO,FX,0.00001 !Convergence value
FSCO,FY,0.00001 ! " "
FSCO,FZ,0.00001 !
FSCO,UX,0.00001
FSCO,UY,0.00001
FSCO,UZ,0.00001

!Output Frequency
FSOU,ALL !Write each iteration

!Relaxation Value
FSRE,ALL,0.6 !Set relaxation value

ALLSEL,ALL
SAVE

!Are we solving it this time?
*IF,c_SOLV,EQ,0,THEN
    FINISH
    /EXIT
    /EOF
*ENDIF
FINISH
/COM ... Step 5.0 - Solution.................................

/SOLUTION

/COM ... Step 5.1 - Define Monitor File DOFs............... 

!Select node at the top center of the biofilm:
ESEL,S,TYPE,,2 !Select all type 2 elements
NSLE,S !Select all nodes with ^
n_top = NODE(0,0,(lc_h+tc_h)/2)
n_lead = NODE(cx,0,l_h)
n_trail = NODE(fx,0,t_h)

!Define monitored DOF's (Monitor,1 is the default - CPU time)
MONITOR,2,n_top,UX !Tracks X-displacement
MONITOR,3,n_top,UY !Tracks Y-displacement
MONITOR,4,n_top,UZ !Tracks Z-displacement
MONITOR,5,n_lead,UX !Tracks X-displacement
MONITOR,6,n_lead,UY !Tracks Y-displacement
MONITOR,7,n_lead,UZ !Tracks Z-displacement
MONITOR,8,n_trail,UX !Tracks X-displacement
MONITOR,9,n_trail,UY !Tracks Y-displacement
MONITOR,10,n_trail,UZ !Tracks Z-displacement

/COM ... Step 5.2 - Label Nodes For Observation............

n_leadbase = NODE(cx,0,0) !Label node at base of leading edge
n_trailbase = NODE(fx,0,0) !Label node at base of trailing edge
n_trailtop = NODE(fx,0,t_h) !Label node at top of trailing edge

/COM ... Step 5.3 - Solve Model..............................

ALLSEL,ALL
SAVE

ALLSEL,ALL
SOLVE !Are you serious?

FINISH

/COM ... Step 6.0 - Post Processing........................
/POST1  !Enter post processor

/COM ... Step 6.1 - Set View.............................................

ALLSEL, ALL

!Call up results
RESUME,%m_job%,db
INRES, ALL  !Identifies that all data be retrieved
FILE,%m_job%,rst  !File name from which data is retrieved
SET, LAST  !Reads last set from *.rst file.
ALLSEL, ALL

! Set View Preferences
ESEL, S, TYPE,, 2  !Select material type 2 only (Fluid won't plot)
/DSCALE, ALL, 1.0  !Displacement scaling = 1:1 (True scale)
INRES, ALL  !Get all structural data
FILE  !Structural file location (Above)
SET, LAST  !Load last set
/VIEW, 1, 0, -1, 0  !View from -Y axis
/FOC, 1, 0, 0, 0  !Center on Origin
/DIST, 1, 0, 0.5  !Zoom scale
PLNSOL, S, EQV, 2  !Plot Von Mises Stress

/COM ... Step 6.2 - Prony Series Parameter File..................

!Create name for file, and record Prony Series Parameters
p_filename = STRCAT(m_job,'_prony')  !Builds file name: *._prony
*CFOOPEN,%p_filename%,txt  !creates text file
*VWRITE,s_E0,s PR
(2X,'E0:',F16.8,2X,'PR:',F16.8)
*VWRITE,s_A1,s TAU1
(2X,'A1:',F16.8,2X,'TAU1:',F16.8)
*VWRITE,s_A2,s TAU2
(2X,'A2:',F16.8,2X,'TAU2:',F16.8)
*VWRITE,G1,h1,G2,h2
(2X,'G1:',F16.8,2X,'h1:',F16.8,2X,'G2:',F16.8,2X,'h2:',F16.8)
*CFCLOS

/COM ... Step 6.3 - Resultant Surface Force Calculation...........

!Load Results
RESUME,%m_job%,db
INRES, ALL
FILE, %m_job%, rfl

p_NumSets = NINT(c_Time)  !# of sets in results file

!Define values used in Array
!set#, time, FxP, FzP, FxT, FzT, FxR....
*DIM, p_SetResultant, ARRAY, p_NumSets+1, 11

ALLSEL, ALL
*DO,p_SET,1,p_NumSets,1 !Do, p_NumSets times, at each sec.
SET,NEAR,,,p_Set

!reset variables which change through each loop
!(y-components typically in symmetry)
p_FxR = 0
p_FzR = 0
p_MzR = 0

! select FSI boundary nodes on solid side
ASEL,S,,,201,203,1
ASEL,A,,,301,305,1
ASEL,A,,,401,405,1
ASEL,A,,,501,505,1
ASEL,A,,,604
ASEL,A,,,609
ASEL,A,,,613
NSLA,S,1

!Integrate pressure to calculate FX, FZ, MY
!integrate nodal results for pressure
INTSRF,PRES

! retrieve X component of resultant pressure force
*GET,p_FxP,INTSRF,,PRES,FX

! retrieve Z component of resultant pressure force
*GET,p_FzP,INTSRF,,PRES,FZ

! retrieve Y component of press. moment around origin
*GET,p_MyP,INTSRF,,PRES,MY

! integrate wall shear to calculate FX,FX,MX,MY
!integrate nodal results for wall shear
INTSRF,TAUW

! retrieve X component of resultant wall shear force
*GET,p_FxT,INTSRF,,TAUW,FX

! retrieve Z component of resultant wall shear force
*GET,p_FzT,INTSRF,,TAUW,FZ

! retrieve Y component of wall shear mom. around orig
*GET,p_MyT,INTSRF,,TAUW,MY

! add to calculate resultant FX,FX,MX,MY
!resultant of shear and pressure in x dir
p_FxR = p_FxP + p_FxT

!resultant of shear and pressure in z dir
p_FzR = p_FzP + p_FzT
! resultant of moment around y axis
p_MyR = p_MyP + p_MyT

! write set resultant to array
p_SetResultant(p_Set,1) = p_Set/c_dtFSI  ! set number
p_SetResultant(p_Set,2) = p_Set        ! time
p_SetResultant(p_Set,3) = p_FxP        ! Pressure force in x
p_SetResultant(p_Set,4) = p_FzP        ! Pressure force in z
p_SetResultant(p_Set,5) = p_FxT        ! Shear force in x
p_SetResultant(p_Set,6) = p_FzT        ! Shear force in z
p_SetResultant(p_Set,7) = p_FxR        ! Resultant force in x
p_SetResultant(p_Set,8) = p_FzR        ! Resultant force in z
p_SetResultant(p_Set,9) = p_MyP        ! Pressure moment in y
p_SetResultant(p_Set,10) = p_MyT       ! Shear moment in y
p_SetResultant(p_Set,11) = p_MyR       ! Resultant moment in y

*ENDDO

! write out array of resultants by data set
p_filename = STRCAT(m_job,'_resultant')
*CFOPEN,%p_filename%,txt
*VWRITE,p_SetResultant(1,1),p_SetResultant(1,2),p_SetResultant(1,3),...
p_SetResultant(1,4),p_SetResultant(1,5),p_SetResultant(1,6),...
p_SetResultant(1,7),p_SetResultant(1,8),p_SetResultant(1,9),...
p_SetResultant(1,10),p_SetResultant(1,11)

(2X,F6.1,'   ',F8.3,'   PresX: ',E16.10,'   PresZ: ',E16.10,'   ...
ShearX: ',E16.10,'   ShearZ: ',E16.10,'   ResFX: ',E16.10,'   ...
ResFZ: ',E16.10,'   PresMY: ',E16.10,'   ShearMY: ',E16.10,'   ...
ResMY: ',E16.10)
*CFCLOSE

/COM ... Step 6.4 - Stress at Certain Nodes.........................

! Define file to report stress in the following nodes:
! (Nodes were defined in step 5.2, above.)
!   Node "A"
!n_leadbase = NODE(cx,0,0)  ! Label node at base of leading edge
!   Node "B"
!n_trailbase = NODE(fx,0,0)  ! Label node at base of trailing edge
!   Node "C"
!n_trailtop = NODE(fx,0,t_h)  ! Label node at top of trailing edge
! Load Results
RESUME,%m_job%,db
INRES,ALL
FILE,%m_job%,rst

! number of sets in results file
p_numSets = NINT(c_Time)

! set#, time, A Stress, B Stress, C Stress
*DIM,p_SetStress,ARRAY,p_numSets+1,5

ALLSEL,ALL

*DO,p_Set,1,p_numSets,1
  SET,NEAR,,,,p_Set ! set to be read
  !(Nearest data set to time)
  !Get value from nodes...
  !VonMises Stress from leading base
  *GET,p_nLead,NODE,n_leadbase,S,EQV
  !VonMises Stress from trailing base
  *GET,p_nTrail,NODE,n_trailbase,S,EQV
  !VonMises Stress from trailing top
  *GET,p_nTop,NODE,n_trailtop,S,EQV
  p_SetStress(p_Set,1) = p_Set/c_dtFSI ! Set number
  p_SetStress(p_Set,2) = p_Set ! Time
  p_SetStress(p_Set,3) = p_nLead ! Leading edge stress
  p_SetStress(p_Set,4) = p_nTrail ! Trailing edge stress
  p_SetStress(p_Set,5) = p_nTop ! Top trailing stress
*ENDDO
!Create name for file, and record Maximum Stress at said nodes

p_filename = STRCAT(m_job,'_Stress')!Builds file name: *_Stress
*CFOPEN,%p_filename%,txt!creates text file
*VWRITE,p_SetStress(1,1),p_SetStress(1,2),p_SetStress(1,3), ...
p_SetStress(1,4),p_SetStress(1,5)

/COM ... Step 6.5 - Maximum Stress .................................

!Load Results
RESUME,%m_job%,db
INRES,ALL
FILE,%m_job%,rst

! number of sets in results file
p_numSets = NINT(c_Time)

! set#, time, Max
*DIM,p_SetMax,ARRAY,p_numSets+1,3

ALLSEL,ALL

*DO,p_Set,1,p_numSets,1
  SET,NEAR,,,,p_Set ! set to be read
  !(Nearest data set to time)
  !Plot Von Mises Stress
  PLNSOL,S,EQV,2 !Will call up max value from plot
  ! Get maximum stress value for that time set
  *GET,p_nMaxVon,PLNSOL,0,MAX

  p_SetMax(p_Set,1) = p_Set/c_dtFSI ! set number
  p_SetMax(p_Set,2) = p_Set ! time
  p_SetMax(p_Set,3) = p_nMaxVon !Maximum Von
  !Mises Stress

*ENDDO

!Create name for file, and record Prony Series Parameters

p_filename = STRCAT(m_job,'_maxVon')!Builds file name: *_maxVon
*CFOPEN,%p_filename%,txt!creates text file
*VWRITE,p_SetMax(1,1),p_SetMax(1,2),p_SetMax(1,3)
(2X,F6.1,' Time: ',F8.3,' Max V.M. Stress: ',E16.10)

FINISH

/EOF

/COM ... End of File .............................................WOW...