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Computational modelling of fluid-porous solid interaction systems

Goodarz khodabakhshi

A Doctoral thesis submitted in partial fulfilment of the requirements for the award of the Doctor Philosophy Degree of Loughborough University

December 2007
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ABSTRACT

Deformation of a porous medium due to the pressure applied by an interacting fluid passing through it is a phenomenon which occurs in a number of applications such as filtration and membrane separation processes. Mathematical modelling of these systems using porous medium theory has proved to be beneficial in the design of experiments and equipments as well as gaining better insight about multi-physics phenomenon such as combined fluid flow and solid deformation regimes.

In the present work the interaction of fluid and porous solid medium has been studied. The governing partial differential equations representing porous solid deformation and fluid flow have been solved simultaneously. A nodal replacement technique has been developed for the direct linking of fluid and solid regimes which removes any need for the specification of additional constraints at the interface between solid and fluid domains. To cope with complex geometries and when the nonlinearity of processes involved, flexible finite element schemes have been constructed.

It is shown that the developed techniques generate accurate and stable results for the combined fluid/solid modelling resolving problems such as numerical locking unified stabilization for both solid and fluid equations and prevents 'numerical locking'. A number of numerical tests has been conducted which show that the developed model is capable of yielding theoretically expected and accurate simulations for realistic industrially relevant problems.

Key words: Fluid-solid porous, interaction, porous medium, stress analysis, finite element analysis
List of symbols

$u_x$ velocity in x direction
$u_y$ velocity in y direction
$u$ velocity
$p$ pressure
$u$ displacement in x direction
$v$ displacement in y direction
$\eta$ viscosity
$p$ density
$k$ permeability
$E$ young's modulus
$V$ Poisson's ratio
$g$ body force per unit volume of fluid
$\sigma$ Cauchy stress tensor
$N$ shape function
$M$ reduced shape function
$\epsilon$ porosity
$w$ weight function (test function)
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Introduction

Analysis of multiphysics problems, and in particular, the simulation of fluid-solid interactions, has been the focus of intensive research in recent years. This is mainly because that numerical methods provide powerful and computationally efficient modern techniques for the solution of complex engineering problems. Traditionally iterative techniques have been used to combine the simulation of conjunctive fluid solid problems. However, there are many problems in which a direct (fully coupled) analysis is needed to model a fluid-solid problem accurately.

Currently there are two numerical techniques for conjunctive simulation of fluid-solid interactions. These are directly coupled and sequentially coupled methods. Many commercial FEA codes use either direct or sequential approaches.

In directly coupled analysis working equations of the numerical scheme assemble all of the physical field unknowns in one matrix and solve it as a whole. In sequential coupling (often referred to as load-vector or staggered coupling), the working equations of one unknown field are partially solved and the results are passed as loads to the other field.

Deformation of porous media due to the pressure applied by flowing fluid passing through it is a challenging fluid/solid interaction problem. This phenomenon occurs in a number of industrially relevant applications such as filtration and membrane separation processes. The main aim of this research has been the modelling of fluid flow through porous media. As the fluid flows through a porous system it interacts with the porous structure and hence the combined system should be viewed as a conjunctive fluid flow-solid deformation problem. Mathematical modeling of fluid flow through a porous medium is hence required to predict the deformation of the solid system and its consequences. In the case of porous media the deformation analysis of the solid structure should be known in order to maintain the serviceability of the medium, which must remain functional for its intended use under routine loadings.
Objectives of the project

To achieve the stated aim of the present research, the following objectives were fulfilled:

1. A novel nodal replacement technique has been developed for the direct linking of the fluid flow equations in free domain (Stokes equation) to the equation of fluid flow in porous medium (Darcy equation). This method is also applied to link the equations of fluid flow and solid deformation. This method removes the need for any additional constraints at the interface between the fluid regimes (i.e. free/porous flow) or solid and fluid domains. Finite element technique offers the best way to apply the stated scheme to geometrically complex domains.

2. A filter design strategy through definition of the stresses and deformations of porous media under working conditions. The predicted failure criterion provides a chance to assess the suitability of a filter for a given process.

3. Computational prediction of fluid variables and the functional relationships between them. Such information results in the improvements of existing operations and can be used as a design tool.

4. Development of a technique that generates unified stabilization for both solid and fluid equations and prevents ‘numerical locking’ whilst preserving the geometrical flexibility of the computational grid.
Thesis outline

The present thesis has 6 chapters with additional sections for appendices and a references section. In what follows a brief review of each chapter is given.

1-Introduction
The subject and aim of the present study and its significance are discussed. The tasks involved in achieving the overall objectives of this study are clearly outlined.

2-Litreature survey
This section contains a review of studies carried out by various researchers in the field of solid-fluid interactions. Different types of methods used to solve the fluid-solid interaction problems have been described.

3-Mathematical model
The governing equations for fluid flow, solid and porous solid deformation are given and the significances of the individual terms involved are discussed. The basic assumptions made to derive these equations and their validity are also discussed. The prescribed boundary conditions for each set of equations have been described.

4-Numerical schemes
Following the discussion of the governing equations in chapter 3, the numerical techniques used in this study to solve these equations are explained. Two different types of solutions are discussed. The final working equations for each solution scheme are presented.

5-Results and discussion
The modelling procedure developed in chapter 4, has been used to solve a number of problems. This chapter provides a comprehensive explanation of the benchmark problems and results obtained.

6-Conclusions
This chapter consists of concluding remarks that are drawn from the simulation results. A list of suggestions for future works is given at the end of this chapter.

References

Appendices

1- Arbitrary-Lagrangian -Eulerian (ALE) method
2- Stress analysis in solid.
3- List of published papers.
4- Program listing and sample input and output file.
2.1 Introduction

Many systems in engineering present a degree of interaction or coupling between fluids and structures. Fluids such as water, air, or lubricants may be interacting with solid elements in buildings, dams, offshore structures, mechanical components, pressure vessels, etc.

In fluid-structure interaction analyses, forces generated within the fluid domain affect the solid part while solid deformation changes the fluid regime. For most interaction problems, the computational domain is divided into a fluid part and a solid part. The interaction occurs along the interface of the two domains. By having the two models coupled, we can perform simulations and predictions of many physical phenomena.

A typical fluid-structure interaction problem is illustrated in Figure 2-1. The fluid flow model is defined in the fluid domain with wall boundary conditions, prescribed velocity at the inlet, zero distributed normal-traction at the outlet and, most importantly, the fluid-structure interface condition. The solid model is defined in the structural domain, where its bottom is fixed and its top is the fluid-structure interface. The typical task of an analysis of a fluid-structure model is to obtain the fluid and structure response through the coupled solution. The structural model is based on a Lagrangian coordinate system and the displacements are the primary unknowns. A pure fluid model is always analyzed using an Eulerian coordinate system. However, for fluid-structure interaction problems, the fluid model must be based on an arbitrary-Lagrangian-Eulerian coordinate system since the fluid-structure interface is deformable. Therefore, the solution variables of the fluid flow include the usual fluid variables (pressure, velocity, etc.) as well as displacements.
A survey of various types of fluid-solid system is shown in Figure 2.2. Moving in the chart (Figure 2.2) from left to right sections, the complexity of the problems increases.
Based on the physical nature of the fluid-solid interaction system, the fluid and solid can be coupled in either of the following ways:

- **Two-way fluid-structure coupling**
  For many coupled problems, the fluid traction affects the structural deformations and the solid displacement affects the flow pattern. This fact is the reason for performing fluid-structure interaction analyses. This type of analysis is called two-way coupling.

- **One-way fluid-structure coupling**
  In certain cases, the deformation of the solid is so small that its influence on the fluid flow is negligible. Then only the fluid stress needs to be applied onto the structure and no iteration between the fluid and solid models is needed. This type of interaction, is called one-way coupling. Typical examples of this behaviour are wind forces on stiff buildings or hydrodynamic forces on massive offshore platforms.
To reach solution effectiveness, the coupled system can be either directly or iteratively solved.

2.1.1 Iterative computation used in two-way coupling

This computing method is also called the partitioned method. In this solution, the fluid and solid solution variables are fully coupled. The fluid equations and the solid equations are solved individually in succession, always using the latest information provided from another part of the coupled system. This iteration is continued until convergence in the solution of the coupled equations is reached.

Teixeira et al [1] proposed an algorithm to simulate fluid-solid interaction problems using a partitioned scheme. A two-step explicit Taylor-Galerkin scheme, with linear tetrahedral finite elements is employed. The structure is analyzed using generalized conforming triangular plates and shell elements. The New-mark method is employed to integrate in time the dynamic equilibrium equation. The non-linear and the algebraic systems are solved using an incremental-iterative scheme and conjugate gradient method, respectively. Feng [2, 3] developed the heterogeneous finite element method for fluid-solid interaction model. The heterogeneous method (in space) consists of standard Galerkin finite element discretization in the fluid region and mixed finite element discretizations in the solid region which simultaneously approximate the stress and displacement variables. Explicitly building one of the two interface conditions into the finite element spaces would solve the difficulty of establishing the optimal order error estimates which is caused by the interface conditions between solid and the fluid on their contact surface.

One of the major difficulties in the application of finite element methods to fluid and fluid-structure interaction is to find an effective discretization procedure for the convective terms as well as the diffusion terms, i.e. for low Reynolds number flows, the stability (inf-sup) condition must be satisfied; and for high Reynolds number flows, effective up-winding techniques have to be used. Therefore, it is highly desirable to have a procedure for combining up-winding schemes with the mixed elements that satisfy the stability (inf-sup) condition. Bathe et al. [4] introduce an up-
winding scheme with the mixed elements for the low order 4-node velocity, 3-node continuous pressure triangular element, which satisfies the stability (inf-sup) condition. A mixed up-winding procedure based on a control volume up-winding discretization for the convection terms and standard Galerkin discretization for the diffusion terms was proposed and confirmed to be reliable in various fluid flow and fluid-solid interaction problems [5]. For the convection term, each two dimensional, second order 9-noded element is split into four 4-noded elements while adopting a control volume up-winding finite element discretization and for other terms, the traditional 9-noded mixed elements which satisfy the stability (inf-sup) condition can be used [6].

The method that has emerged during the last few years employ different approximations in fluid and solid domains, typically finite difference or volume methods for fluid and finite element for solid. Fluid and solid are thus coupled after discretization since coupling is achieved after numerical approximation.

2.1.1.1 Information Transfer

For the information transfer FSI computations require that pressure loads are transmitted from the fluid side of the fluid-structure interface to the structural nodes on that interface. Also, once the motion of the structure has been determined, the motion of the fluid mesh points on the interface has to be imposed. In FSI simulations generating matching meshes at the fluid-structure interface is usually not desirable, because the flow generally requires a much finer mesh than the structure and, due to the modularity of the partitioned coupling technique, different teams may take care of different solvers. When meshes are non-matching, an interpolation/projection step has to be carried out to enable transfer of information between the two domains. In the literature different ways can be found to transfer data between non-matching meshes, such as nearest neighbour interpolation, projection methods and methods based on interpolation by splines.
There are several criteria which should ideally be satisfied for such a data exchange or coupling method. The most important are: (i) global conservation of energy over the interface, (ii) global conservation of load over the interface, (iii) accuracy, (iv) conservation of the order of the coupled solvers and (v) efficiency, which is defined as a ratio between accuracy and computational costs.

The simplest and fastest way to perform the information transfer is to obtain the information from the closest point in the other mesh, the so called nearest neighbour interpolation [7]. A more accurate way of handling the data transfer is by projection. To obtain information from the other mesh, a point can be orthogonally projected on that mesh and the information in that projection point can be used in the original point. This technique can be exploited when Gauss integration is in used in the calculation of integrals over the interface and is commonly used to perform solid-fluid interaction calculations. This method is implemented in the commercial coupling library MpCCI [8]. The third way to exchange data is to use spline based methods. These are often applied in interpolation schemes in finite element methods, in the computer graphics world and in medical imaging.

2.1.2 Direct computation used in two-way coupling

This computing method is also called the simultaneous solution method. In this direct solution method, as in the above iterative solution, the fluid and solid solution variables are also fully coupled. The fluid equations and the solid equations are combined and treated in one system. Therefore, they are linearized in a matrix system, as for a fluid model or a solid model alone.

Omar and Li [9] considered the problem of the interaction of stationary viscous fluid with an elastic solid that undergoes large displacement. The fluid is modelled by the stationary incompressible Navier-Stockes equation in an Eulerian frame of reference, while a Lagrangian reference frame and large displacement-small strain theory is used for the solid. The variational formulation is approximated by the Galerkin finite element method, yielding a system of non-linear algebraic equations in unknown fluid velocities and pressures and solid displacements. A Newton-like method is introduced for solution of the discrete system. The method employs a modified Jacobian that
enables decomposition into separate fluid and solid sub-domains. This domain decomposition avoids the possible ill conditioning of the Jacobian, as well as the need to compute and store geometric coupling terms between fluid and interface shape.

The size of the coupled fluid-structure interaction problem is generally large. Many researchers have attempted to reduce the problem size in different ways. Seybert [10] employed Ritz Vectors and Eigenvectors along with the combination of finite element and boundary element methods to reduce the problem size.

Since the variational principals are employed to derive numerical solutions, many researchers have attempted to derive variational principals for different classes of fluid-structure interaction problems. In [11], a coupled system of potential and wave equations was considered. Elementary fluid interaction with a rigid cavity or a moving wall were studied in [12] and with an elastic solid in [13]. Interactions between linearized inviscid fluid (e.g. Euler equation) and elastic solids were analysed in [14,15]. An algorithm applicable to an inviscid nonlinear fluid, coupled with rigid walls was given in [16]. There is an extensive literature on linearized viscous fluid coupled with solids. Solid modelled by plate equations or shell equations were treated in [17, 18, 19, 20]. The Stokes equations coupled with a beam equation was analysed in [21]. In [22, 23], interactions between a linearized viscous fluid and elastic solid were studied. [24] discussed the same interactions with rigid walls. There is also a vast literature on fluid-structure interaction for which the fluid is modelled by non-linear viscous fluid models. Rigid body motions of solid in a non-linear viscous fluid were studied in [25, 26, 27, 28]. In [29], the Navier-Stokes equations coupled to the plate equations were studied. The work of [25, 30, 31, 32] treated interactions between non-linear viscous fluids and elastic solids. In the majority of the previous cited references the solid model of lower spatial dimension was used. In [22], the homogenisation of mathematical model for the Stokes equation coupled to the equations of linear elasticity was considered. Both existence of a solution and numerical experiments for a problem in which a nonlinear viscous fluid is coupled to an elastic solid in one dimension were discussed in [30]. Due et al [33] developed a time dependent system modelling the interaction between a fluid following Stokes equation and an elastic structure. A divergence-free weak formulation is introduced
which does not involve the fluid pressure field. The existence and uniqueness of a weak solution is proposed. Liu [34] presented a general variational principle for fluid-solid interaction problems with sloshing.

2.1.3 Direct computation used in one-way coupling

In this case, the fluid stress is applied onto the structure while the structure has no influence on the flow field.

2.2 Mesh-less method for fluid solid interaction problems

Generally, simulation of incompressible fluid flow has been based on the Eulerian formulation of the fluid mechanics equations. However, it is difficult to analyse problems in which the shape of the interface changes continuously or in fluid-structure interactions with free-surface, where geometrically complex problems are involved. More recently, particle methods in which each fluid particle is followed in a Lagrangean manner have been used [35]. On the other hand, a family of methods called mesh-less methods have been developed both for structural, and fluid mechanics problems. All these methods use the idea of a polynomial interpolant that fits the number of points minimizing the distance between the interpolated function and the value of unknown point. Lately, the mesh-less ideas were generalized to take into account the finite element type approximations in order to obtain the same computing time in mesh generation as in the evaluation of mesh-less connectivities. Smoothed particle hydrodynamics (SPH) technique is a mesh-less method which has been used for simulation of fluid-structure systems. The SPH method works by dividing the fluid into a set of discrete "fluid elements". These particles have a spatial distance (known as the "smoothing length", typically represented in equations by $h$), over which their properties are "smoothed" by a kernel function. [36]. This means that any physical quantity of any particle can be obtained by summing the relevant properties of all the particles which lie within two smoothing lengths. For example, the temperature of particle $i$ depends on the temperatures of all the particles within a radial distance $2h$ of particle $i$. The contributions of each particle to a property are
weighted according to their distance from the particle of interest. Mathematically, this is governed by the kernel function (symbol \( W \)). Kernel functions commonly used include the Gaussian function and the cubic spline. The latter function is exactly zero for particles further away than two smoothing lengths (unlike the Gaussian, where there is a small contribution at any finite distance away). This has the advantage of significantly reduced computational effort by not including the relatively minor contributions from distant particles. The equation for any quantity \( A \) of particle \( i \), represented as \( A_i \) is given by the equation

\[
A_i(r) = \sum_j m_j \frac{A_j}{\rho_j} W(r_i - r_j, h)
\]  

(2-1)

where \( m_j \) is the mass of particle \( j \), \( A_j \) is the value of the quantity \( A \) for particle \( j \), \( \rho_j \) is the density associated with particle \( j \), \( r \) denotes position and \( W \) is the kernel function mentioned above.

Recently Idelson et al. [37] proposed a new method to approach FSI problems. Unified Lagrangian formulation has been used for both solid and fluid domains. This basically means that the analysis domain, containing both fluid and solid sub-domains which interact with each other, is seen as a single continuum domain with different material properties assigned to each of the interacting sub-domains. This approach makes no distinction between fluids and solids for the numerical solution and single computer code can be used for solving the FSI problem. Classical stabilization terms used in the momentum equations are unnecessary due to the lack of convective terms in the Lagrangian formulation. Furthermore, the Lagrangian formulation simplifies the connection with fixed or moving solid structures, thus providing a very easy way to solve fluid-structure interaction problems. The governing equations for the fluid and solid domains (in Lagrangian frame of reference) are discretized and solved with the particle finite element method (PFEM). The PFEM treats the mesh nodes in the fluid and solid domains as moving material points which can freely move and even separate from the main fluid domain representing, for instance the effect of water droplets. A finite element mesh connects the nodes defining the discretized domain where the governing equations are solved in the standard FEM fashion. The motion of
the mesh discretizing the total domain (including both fluid and solid domain) is followed during the transient solution.

2.3 Solution strategies

Various solution strategies can be pursued, dealing with fluid-solid interaction problems. In structural analysis, Newton-Raphson iteration is the most effective strategy, in which the resulting matrix equations are solved using either a sparse or an iterative solver. In fluid-flow analysis, successive substitution and Gauss-Seidel type iterative schemes are widely employed, but Newton–Raphson iteration can also be effective. The convergence in the iterations is frequently improved by nondimensionalizing the fluid equations. Using the Newton-Raphson method, the resulting matrix equations are solved with an iterative scheme such as biconjugate gradient technique when the number of fluid equations is very large. A sparse solver is however, more effective if the number of equations considered is not too large.

For the nonlinearities, Newton-Raphson iterations can be used for both the solid and the fluid, while simple successive substitution can be employed for the fluid. For the interface conditions, successive substitution is used with an acceleration scheme. To solve the matrix equations of the fluid and structural domains, sparse solvers or iterative solvers with pre-conditioners (conjugated gradient and multigrid methods for the structure, and biconjugated gradient, GMRES and multigrid method for the fluid) can be used.

2.4 A review of methods used to update the domain geometry

One of the most well-known methods used to capture the interaction between structure and fluid is the Arbitrary Lagrangian Eulerian method (ALE). An Arbitrary Lagrangian Eulerian method allows arbitrary motion of grid/mesh points with respect to their frame of reference by taking the convection of these points into account as described in [38], [39] and [40] and many others thereafter. In the case of an FSI problem, the fluid points at the fluid–solid interface are moved in a Lagrangian manner. Since the method is easy to implement, has low computational cost and is accurate, it is advisable to use this method whenever possible. However, for large
translations and rotations of the solid or inhomogeneous movements of the grid/mesh points fluid elements tend to become ill-shaped, which would have a negative effect on the accuracy of the solution. Re-meshing, in which the whole domain or part of the domain is spatially rediscretised, is then a common strategy. The process of repeated mesh generation during a transient computation can, however, be a very troublesome and time consuming task. Furthermore, the transfer of solutions from the degenerated mesh to the new one may introduce artificial diffusion, causing loss of accuracy.

In contrast to the ALE technique where the fluid–solid interface is accurately captured other types of methods do not require any changes of the fluid mesh/grid. A widely used non-boundary-fitting method for FSI applications is the immersed boundary method, which was proposed by Peskin [41] and [42]. The first models consider a finite difference grid for the fluid domain with an immersed set of non-conforming boundary points that are mutually interconnected by an elastic law. This solid boundary interacts with the fluid by means of local body forces applied to the fluid at the position of the solid points. This body force imposes the kinematic constraint that the velocity at each of these solid points is coupled to the (interpolated) fluid velocity at that point. The introduction of these body forces has become the basic idea behind several non-boundary-fitting FSI methods. Throughout the years, the Immersed Boundary Method has been successfully applied in many application fields [43], [44] [45] and [46].

Another method closely related to the immersed boundary method, is the so-called fictitious domain method [47]. Unlike the immersed boundary method that was developed within a finite difference framework, the fictitious domain method evolved from the field of finite elements. Coupling is established by constraining the fluid and rigid body at their interface using a (distributed) Lagrange multiplier and extending this constraint to the inner body. The fictitious domain method is very similar to the immersed boundary method. The main difference is that through application of the multipliers in the weak form (which represent the body forces), the forces are imposed in a distributed manner using an integral formulation.
Based on the fictitious domain idea Baaijens [48] proposed a fluid-solid interaction version suitable for slender bodies. In his work a fluid and solid mesh are generated independently from each other and both domains are coupled by means of a Lagrange multiplier along the boundary of the solid. The solid is described in a Lagrangian frame of reference, deforming under the fluid forces, while the Eulerian fluid mesh does not require re-meshing. This method has been successfully applied in flexible heart valve simulations [49] and [50].

A disadvantage of Baaijens’ technique is that it is only applicable to slender bodies. Several extended versions have since been proposed where non-slender elastic solid bodies are coupled across the whole body instead of a boundary, thus broadening the application field. The Extended Immersed Boundary Method [51] and the Immersed Finite Element Method [52] describe the solid using the finite element method while the fluid could be formulated using either a finite difference or finite element method, respectively. The coupling is performed using the discrete dirac delta functions that find their origin in meshless methods known as Reproducing Kernel Particle Method (RKPM). Both methods are based on the explicit time integration for the fluid-solid coupling. Examples include the dropping of rigid or deformable particles in a three-dimensional channel. Yu [53] [65] set out his version of the fictitious domain method for non-slender deformable bodies. Analysis of this approach was performed by two numerical examples: the motion of a slender solid slab in a pulsatile flow and the self-sustained flapping of a slender solid in a constant flow. Finally, the immersed continuum method should be mentioned, which computes the motion and deformation of a compressible solid in a compressible fluid [54].

Non-boundary-fitting methods have a reduced accuracy for the solution near the fluid-solid interface due to interpolation errors. Conversely, in the ALE methods the fluid discretisation tends to get highly distorted requiring difficult and expensive re-meshing. Therefore, another variation on the distributed Lagrange multiplier principle was proposed by Van Loon et al. [55]. A combination of the two approaches might lessen their disadvantages without losing too much of the benefits. The approach consisted of the fictitious domain method similar to that of Baaijens, but extended with an ALE step and a local adaptive meshing algorithm for the fluid mesh [56]. Due
to the use of the Lagrange multiplier the meshes do not have to be conforming at the solid-fluid interface, which allows the re-meshing algorithm to be simple and very local. To show the improved accuracy, shear stresses along both sides of the solid were computed. Also, Van De Vosse [57] used arbitrary Lagrange-Euler fictitious domain (ALE-FD) method for fluid-structure interaction problems in cardiovascular and biomechanics applications in terms of weighted residual finite element formulation. For both fluid flow and solid mechanics of vascular tissue, the performance of tetrahedral and hexahedral Crouzeix-Raviart elements were evaluated. The possibilities that are offered by the ALE-FD method were illustrated by means of a simulation of valve dynamics in a simplified left ventricular flow model.

Zhang et al [58] described the recent development of fluid-structure capabilities in the commercial software package ADINA. ADINA is a general-purpose finite element and finite volume code for the analysis of structures, fluid flows and fluid-structure interactions. It has a strong theoretical foundation based on the pioneering work of K.J. Bathe in the field of computational mechanics. His contributions to structural, fluid flows and their interactions are accurately and reliably implemented in the ADINA system. In this case, fluid flow can be modelled as incompressible, slightly compressible or fully compressible. Fluid flow through a porous medium can also be modelled in this case. Structures can be modelled as 2D/3D solids, beams or shells. The response of the structure can be linear or non-linear, and can also include contact effects. The fluid and structure can be coupled through their interface (FSI), porous media (PFSI) or thermal materials (TFSI). Both iterative and direct solution procedures can be used for solving the fully coupled system.

**2.5 Kinematic and dynamic conditions at the interface**

The fundamental conditions applied to the fluid-structure interfaces are the kinematic condition (or displacement compatibility)

\[ u \mid_{\psi} = \Psi \]  \hspace{1cm} (2-1)

and the dynamic condition (or traction equilibrium)
\[ n \tau_f = n \tau_s \]  

(2-2)

where \( d_f \) and \( d_s \) are the fluid and solid displacements and \( \tau_f \) and \( \tau_s \) are the fluid and solid shear stresses, respectively. The underlining denotes that the values are defined on the fluid-structure interfaces only. The fluid velocity condition is resulted from the kinematic condition

\[ \dot{y} = \dot{d}_s \]  

(2-3)

if a no-slip condition is applied, or

\[ n. \dot{v} = n. \dot{d}_s \]  

(2-4)

if a slip condition is applied.

The fluid and solid models are coupled as follows:

The fluid nodal positions on the fluid-structure interfaces are determined by the kinematic conditions. The displacements of the other fluid nodes are determined to preserve the initial mesh quality. The governing equations of fluid flow in their ALE formulations are then solved. In steady-state analyses, the mesh velocities are always set to zero even when the fluid nodal displacements are updated. Accordingly, the fluid velocities on the fluid-structure interfaces are zero.

According to the dynamic conditions, on the other hand, the fluid traction is integrated into fluid force along fluid-structure interfaces and exerted onto the structure node

\[ F(t) = \int h^d \tau_f \, dS \]  

(2-5)

where \( h^d \) is the virtual quantity of the solid displacement.
2.6 Porous media

2.6.1 Porous medium-physical description

Porous materials are classified as those with an internal structure containing voids. They comprise a solid phase containing closed and open pores. Attention is mainly focused on the case where the open pores are filled with one or more fluids, i.e. a multiphase media. In the case of geo-materials, i.e. soil, rock, concrete, the fluids may be water, water vapour and dry air. Soil and rock may also contains gas, oil and/or water. The solid and the fluid usually have relative velocities to each other, and because of this and the existence of different material properties, there is interaction between the constituents. Furthermore, the pore structure has, in general, an extremely complicated geometry which makes the geometrical description of the problem rather difficult. For engineering purposes a substitute model at the macroscopic scale is normally assumed where the interacting constituent are presumed to occupy the entire control space. This distribution is obtained by means of volume fraction concept. Volume fractions are given by the ratio of the volume of the constituent to the volume of the control space. A consequence of the volume fraction concept is that the subtitle constituents have reduced densities. These subtitle continua may be treated via the methods of continuum mechanics.

Two strategies are generally used to arrive at the description of the behaviour of these subtitle continua: one could start either from a macro mechanics or from micromechanics viewpoints. Phenomenological and mixture theory approaches, integrated by the concept of volume fractions, belong to the first strategy. Averaging theories, sometimes called hybrid mixture theories, belong to the second one.

Porous media theory has been of interest to research workers for a considerable time. An extensive review of the history of such porous media theories is given by de Boer[59]. Woltman [60] introduced the concept of volume fractions and Delesse [61] dealt with surface fractions. Fick [62] studied the problem of diffusion of mixtures, Darcy [63] the motion of a liquid in a porous solid, and Stefan [64] the diffusion of gas through a porous diaphragm. Fillunger [65] introduced the concept of effective stresses and studied the problem of uplift, friction and capillary in rigid, liquid-
saturated porous solids. Terzaghi [66] investigated saturated deformable porous solids and also made the use of the effective stress principle. Biot [67,68] developed the phenomenological approach of Terzaghi further and extended it to the three-dimensional case.

Modern mixture theories were developed by Morland [69], Goodman and Cowin [70], Sampaio and William [71] and Bowen [72,73]. Averaging theories where developed by Hasanizadeh and Gray [74] and by Whitaker [75]. Finally a macroscopic thermodynamical approach by Biot's theory was used by Coussy [76].

Consolidation which plays an important role in porous media mechanics has been the subject of many researches. A survey of the literature indicates two main areas where consolidation analysis is extensively applied. The first one is connected with the physical loading of soil layers and has probably received the greater attention. This aspect comprises the transient analysis of footings, pile foundations, soil-structure interaction, embankment, large fill dams, etc.

The second aspect of consolidation, connected with the change of hydraulic equilibrium in a system comprising aquifers and aquitards, has received attention only in recent times when considering the effects of extensive groundwater withdrawal for industrial and agricultural purpose.

In engineering practice, settlements were calculated in most cases using Terzaghi's [66] one-dimensional consolidation theory. More recently Biot's [67,68], three-dimensional theory has been used, based on a linear stress-strain constitutive relationship and also a linear form of Darcy's flow rule. The extensive use of computers and the concomitant development of numerical techniques has made more precise analyses possible. The non-linear behaviour of the skeleton and variation of permeability with strain can now be easily taken into account, if necessary. These possibilities, shift attention from the question of problem solving to the problem of modelling observed phenomena. The eventual aim is to develop the capability for making predictive simulations.
The permeability of a porous medium may be regarded as a measure of the ease with which a fluid will flow through its voids. The magnitude of the permeability is determined by the degree of "openness" of the medium, which would be more formally interpreted by the porosity of the medium and the sizes of the pore presenting its internal structure. The most common expression used to describe the permeability is Darcy's law:

\[ k = -\mu Q / [A \rho g (dh/dz)] \]  

(2-2)

Where \( Q \) is the volume of the fluid discharged per unit of time through the cross-sectional area \( A \), \( \mu \) is the viscosity of the fluid, \( \rho \) is the density of the fluid, \( g \) is the acceleration due to gravity, \( dh/dz \) is the hydraulic gradient in the direction of flow, \( z \).

Another frequently encountered permeability model is the Carman-Kozeny model. This model is sometimes referred to as the hydraulic radius model since it assumes pore diameter to be 4 times the void volume of the medium divided by the pore surface area. It relates the permeability to total porosity and specific surface areas of the pores. The mathematical form of the Carman-Kozeny model is

\[ K = \varepsilon^3 \left[ k_o (L_e / L)^2 (1 - \varepsilon)^2 S^2 \right] \]  

(2-3)

Where \( \varepsilon \) is the total porosity, \( k_o \) is the permeability of an infinitely dilute bed, \( L_e \) is the average path length for flow, \( L \) is the path length, \( S \) is the specific surface area.

Archie's law model relates porosity and permeability using a power-law. This model expressed as

\[ K \propto \varepsilon^m \]  

(2-4)

where \( \varepsilon \) is the total porosity and \( m \) is a constant

There are other relations and models for permeability such as Network model and probabilistic models where their definitions can be found in the literature [77].
2.6.2 Mathematical model of fluid flow and deformation of porous medium

The consolidation problem is usually solved in space by a finite element (FE) technique giving rise to a system of first order differential equations. The solution to these equations is typically addressed by an appropriate time marching scheme. The discretization in the time domain may require variable time steps that may change by several orders of magnitude during the analysis. As a matter of fact, in the early phase of consolidation small time steps are needed to obtain a sufficiently accurate solution, while, as the simulation proceeds, a much larger time steps can be used without great loss of accuracy. Time integration usually performed by the well known $\theta$ method, whose stability and accuracy has been discussed by a number of authors. In particular, Bookers and Small [78] proved that an implicit time integration scheme with $\theta \geq 0.5$ is unconditionally stable even if the sequence of time steps is strictly increasing, while the choice $\theta < 0.5$ is conditionally stable and may require a very small time steps.

The solution to the linear system with a small time step may prove quite difficult and results in an ill-conditioned system of equations due to the large difference between the terms arising from the integration of structural equations and those from the flow equations. A practical way to avoid ill-conditioning is suggested by Reed [79] by the use of a scaling factor to reduce the difference in magnitude of pivotal elements. A suitable value of the scaling factor is provided by Sloan and Aboo [80] who try to equate approximately the size of the diagonal terms of the structural equations with those of the flow equations.

Direct sparse solvers are quite efficient for unsymmetric, non-positive definite matrices; the large dimension of the linear system generated by the FE method in a realistic consolidation problem suggests that iterative methods should be used.

Korsawe et al [81], study the effect of different finite element approaches to the consolidation problem. The standard displacement-pressure formulation discretized by Taylor-Hood finite element pair is compared with a Least-square mixed finite element method. The Least-square method approach introduces finite elements spaces
for the approximation of all the process variables involved in the consolidation model, i.e., the fluid flux, pressure, and stress tensor in addition to displacement field. The computations have shown that the Galerkin finite element method is able to preserve pressure gradients, but it is over estimating effective stresses. The major advantage of the Least-square method is the direct approximation of the variables of primary interest (e.g. stresses) and the availability of a posteriori error estimator for adaptive mesh refinement. Also the Least-square method has an advantage of the explicit approximation of Neumann type boundary conditions. Due to the higher number of DOF for the Least-square method in comparison with the Galerkin method, for identical meshes, the computational cost is larger. A comparison of both methods in terms of computational cost, should however be complemented by consideration of desired accuracy for all field variables.

Ehlers [82] formulate the deformation of a saturated porous media using the Theory of Porous Media (TPM). As the solid and fluid assumed to be incompressible, therefore, the so called point of compaction exists. This deformation state is reached when all pores are closed and any further volume compression is impossible due to the incompressibility constraint of the solid skeleton material. To describe this effect, a new finite elasticity law was developed on the basis of a hyperelastic strain energy function, thus governing the constraint of material incompressibility for the solid material. In the case of finite deformations, the influence of deformation dependent permeability on the solution of a boundary value problem is significant. Therefore, a power function describing the dependency of the Darcy’s permeability parameter or the porosity of the solid skeleton has been introduced.

2.7 Filtration

The filter medium is “any material that, under operating conditions of the filter, is permeable to one or more components of a mixture, solution or suspension, and is impermeable to the retaining components”. The principle role of the medium is to separate particles from the fluid with the minimum consumption energy. To achieve this, the selection of the correct medium takes into account factors such as the permeability of the clean medium and the permeability loss of the medium during use.
Serious loss of permeability may be followed by plugging or blinding of the filter medium and can reduce its life time if an uneconomic filtration rate results. Permeability and particle retention are dependent on the interaction between the medium structure and the shape and size distribution of the particles in the feed suspension.

Many materials in diverse form are used as filter media. These include solid fabrications (e.g. wire wound tubes), metal sheets (e.g. perforated), rigid porous media (e.g. ceramics), cartridges, plastic sheets, membranes, woven fabrics, non woven media, and loose media. Textile, woven or non-woven, is probably the most common industrial filter medium.

Membrane filtration utilises thin sheets of permeable material, made from polymers and materials such as ceramics and metals. Membrane filter media are classified according to the size of their pores: membrane with pore size between 0.1 and 20 μm are used in micro-filtration, between 0.001 and 0.1 μm (molecular weights (MW) of 500 to 500000) in ultra-filtration, and between 200 and 1000 MW in nano-filtration. Membrane filter media are configured into tubular, hollow fibre and sheet formats; sheets may be formed into pleat or tubular filters. Many membranes have an asymmetric structure, composed of a thin skin that acts as the surface filter that is supported by the thicker layer designed to give mechanical integrity to the whole structure; the thickness of the membrane may be from less than 1 μm to several hundred μm.

Micro-filtration membranes can be operated in two ways: 1) as a straight-through filter, known as dead-end filtration, or 2) in cross-flow mode. In dead-end filtration, all of the feed solution is forced through the membrane by an applied pressure. This is illustrated in figure 3-a. Retained particles are collected on or in the membrane. Dead-end filtration requires only the energy necessary to force the fluid through the filter. The dead-end micro-filtration may be in different forms (flat sheet, pleated cartridge, capillary, tube, etc.)
The second way to operate micro-filtration membrane is in cross-flow. In this operational mode, shown in figure 3-b, the fluid to be filtered is pumped across the membrane parallel to its surface. Cross-flow micro-filtration produces two solutions; a clear filtrate and a retentate containing most of the retained particles in the solution. By maintaining a high velocity across the membrane, the retained material is swept off the membrane surface.

**Dead-end filtration**

![Dead-end filtration diagram](image)

**Cross-flow filtration**

![Cross-flow filtration diagram](image)

Figure 2-3 schematic representations of a) dead-end and b) cross-flow operation of micro-filtration membranes [83]

**2.7.1 Design considerations**

The optimum design of a micro-filtration membrane system depends on a number of parameters and on the characteristics of the feed stream to be treated. Two important design considerations are 1) the choice of operational mode, either dead-end or cross-flow, and 2) module design.
2.7.1.1 Dead-end vs. cross-flow operation

One important characteristic of a feed stream is the level of solids that must be retained by the micro-filter. The higher the level of solids, the higher the likelihood that cross-flow filtration will be used.

2.7.1.2 Module design consideration

For the membrane to be a useful device, it must be packed in a way that permits the membrane to operate efficiently. Many types of membrane holders and devices are available.

2.7.1.3 Dead-end filter housings

**Disk holders:** Disk holders represent the simplest membrane filter housing, and their design has evolved slowly since their introduction in the 1950s. The membrane is fitted between two plates, a porous one on which the membrane filter is supported, and a feed plate containing a cavity to permit the fluid to contact the membrane freely. The devices are usually plastic or stainless steel, and membrane is usually sealed with an O-ring.

**Pleated cartridges:** Many membranes are pleated, and then formed into a cylinder, substantially increasing the membrane area that can be fit into a given volume. The devices resemble the familiar automotive air filter. End caps are generally attached using curable liquid and melt sealants. Cartridges are then fitted into housings, either as one unit or in groups. The housings are simple pressure vessels, although their design may become elaborate.

**Dead-end spiral:** Spiral-wound modules are popular cross-flow devices, widely used in reverse osmosis and ultrafiltration. A hybrid cross-flow/dead-end filter is being manufactured for microfiltration using the principle of running a spiral-wound module as a dead-end filter. During initial operation, until significant solids have been built up, most of the feed passes along the membrane, becoming dead-ended only near the outlet of the sealed spiral device. When filled with solids, the spiral operates totally as a dead-end filter.
2.7.1.4 Cross flow device

When significant quantities of solid are present, cross-flow operation gives the highest output per unit membrane area. The simplest cross-flow device is a membrane formed inside a tube made from strong, porous material. The feed runs down the inside of the tube, under pressure. Permeate passes through the membrane, then through the porous support.

2.7.2 Darcy's law in filtration (or in any types of low permeability porous flow)

In filtration, Darcy's law is often used in a modified form, where the specific resistance ($\alpha$) replaces the permeability ($k$) and pressure gradient ($dp/dz$) is replaced by the pressure loss per unit mass of solid deposited ($dp/dw$) on the medium:

$$ u = -\frac{1}{\mu\alpha} \frac{dp}{dw} \quad (2-5) $$

where $w$ is the mass of dry cake per unit filter area deposited within distance $z$ from the filter medium. $dw$ and $dz$ are related by:

$$ dw = \rho_s (1 - \varepsilon) dz \quad (2-6) $$

And the total mass of solids deposited is related to the cake thickness (which is important to the design, specification and operation of a filter) by:

$$ w = \rho_s (1 - \varepsilon) L \quad (2-7) $$

$k$ and $\alpha$ are related by:

$$ k = \frac{1}{\rho_s (1 - \varepsilon) \alpha} $$

In general, $\alpha$ varies less than $k$ with pressure and it is therefore used as a primary parameter for the scale-up of filtration equipment. It is not universal, but most
approaches to process design and scale-up use parameters that can be shown to have some equivalence to $\alpha$. 
Chapter 3 Mathematical model

3-1 Basic equations of solids deformation

If a body is in equilibrium under specified static loads, the reactive forces and momentum developed at the support points must balance the externally applied forces and moments. This lead to the following internal equations for a three dimensional body.

(a) equilibrium equations

\[
\begin{align*}
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + \Phi_x &= 0 \\
\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + \Phi_y &= 0 \\
\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + \Phi_z &= 0
\end{align*}
\]  

(3-1)

\(\Phi_x, \Phi_y, \Phi_z\) are body forces per unit volume acting along the directions x, y and z.

(b) stress-strain relation (constitutive relations)

For linearly static isotropic 3-D solid, the stress-strain relations are given by Hooke’s law:

\[
\bar{\sigma} = \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{xz} \\ \sigma_{yz} \end{bmatrix} = [D](\bar{\varepsilon} - \bar{\varepsilon}_0)  
\]

(3-2)

where \(\bar{\sigma}, \bar{\varepsilon}\) and \(\bar{\varepsilon}_0\) are stress tensor, strain vector and vector of initial strain, respectively. The [D] matrix is given by:
where $E$ and $\nu$ are elastic modulus and Poisson's ratio, respectively.

In the case of two-dimensional problems, two types of stress distributions, namely plane stress and plane strain, are possible.

### 3.1.1 Plane stress

The assumption of plane stress is applicable for bodies whose dimensions are very small in one of the coordinate directions. Thus, the analysis of thin plates loaded in the plane of the plate can be made using assumption of plane stress. In plane stress distribution, it is assumed that

$$\sigma_{zz} = \sigma_{xx} = \sigma_{yx} = 0$$  \hspace{1cm} (3-4)

where \( z \) represents the direction perpendicular to the plane of the plate. In this case the matrix \([D]\) reduce to

$$[D] = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}$$  \hspace{1cm} (3-3)
3.1.2 Plane strain

The assumption of plane strain is applicable for bodies that are long and whose geometry and loading do not vary significantly in the longitudinal Z direction. Thus, the analysis of dams, cylinders, and retaining walls can be made using the assumption of plane strain. In plane strain distribution, it is assumed that \( w=0 \) and \( \frac{\partial w}{\partial z} = 0 \) at every cross section. Here, the dependent variables are assumed to be functions of only the x and y coordinates provided we consider a cross section of the body away from the ends. In this case the matrix \([D]\) is reduced to

\[
[D] = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix}
1-\nu & \nu & 0 \\
\nu & 1-\nu & 0 \\
0 & 0 & \frac{1-2\nu}{2}
\end{bmatrix}
\]  

(3-6)

The component of stress in the z direction will be nonzero and will be given by

\[
\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})
\]

(3-7)

and

\[
\sigma_{yz} = \sigma_{zy} = 0
\]

(3-8)

3-1-3 Compatibility equation

When a body is continuous before deformation, it should remain continuous after deformation. In other words, no cracks or gaps should be appearing in the body and no part should overlap another due to deformation. Thus, the displacement should be continuous as well as single-valued. This is known as the “condition of compatibility.”

In the case of two dimensional plane strain problems, the following equation is arisen
for plane stress problems, the following equation is resulted:

\[
\frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = \frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y} \tag{3-10}
\]

In the case of one-dimensional problem, the condition of compatibility will be automatically satisfied.

### 3-1-4 Mathematical modelling of solid deformation

Solid and structural mechanics can be formulated according to two methods: differential equation method and variational method. Hence, the finite element equations can be derived by using either a differential equation method (e.g., Galerkin approach) or variational method (e.g., Rayleigh-Ritz approach). In the case of solid and structural mechanics problems, each of the differential and variational formulation methods can be classified into different categories.

#### 3.1.4.1 Differential equation formulation methods:

a. Displacement method

b. Force method

c. Displacement-force method (mixed method)

d. Weighted residual method

#### 3.1.4.2 Variational formulation methods:

a. Principle of minimum potential energy

b. Principle of minimum complementary energy

c. Principle of stationary Reissner energy
Displacement method

By substituting, first, the displacement, from the strain-displacement relations into stress-strain relation, the stresses will be obtained in terms of displacements. Then by substituting the resultant equations in the equilibrium equations, three equilibrium equations in terms of displacement will be obtained. Now these equilibrium equations can be solved for displacements. Of course, additional requirements such as boundary and compatibility conditions also have to be satisfied while finding the solution for displacement. Since the displacements are made the final unknowns, the method is known as displacement method.

3.2 Mathematical model for plane elasticity deformation

Based on the above explained method (displacement method), the governing equations of elastic solid deformation in general form are derived by substituting the equations (3-2) and (3-3) into equation (3-1). The resultant equations are as follows:

\[
\begin{align*}
- \frac{\partial}{\partial x} \left( c_{11} \frac{\partial u}{\partial x} + c_{12} \frac{\partial v}{\partial y} \right) - c_{33} \frac{\partial}{\partial y} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) &= f_x \\
- c_{33} \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) - \frac{\partial}{\partial y} \left( c_{12} \frac{\partial u}{\partial x} + c_{22} \frac{\partial v}{\partial y} \right) &= f_y
\end{align*}
\]  
\[
\begin{align*}
t_x &= \left( c_{11} \frac{\partial u}{\partial x} + c_{12} \frac{\partial v}{\partial y} \right) n_x + c_{33} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) n_y \\
t_y &= c_{33} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) n_x + \left( c_{12} \frac{\partial u}{\partial x} + c_{22} \frac{\partial v}{\partial y} \right) n_y
\end{align*}
\]

where

\[
c_{11} = c_{22} = \frac{E}{1-\nu^2}, \quad c_{12} = \frac{\nu E}{1-\nu^2}, \quad c_{33} = \frac{E}{2(1+\nu)}
\] 
plane stress

\[(3-11)\]
\[(3-12)\]
Chapter 3 Mathematical model

\[ e_{11} = e_{22} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}, \quad e_{12} = \frac{\nu E}{(1+\nu)(1-2\nu)}, \quad e_{33} = \frac{E}{2(1+\nu)} \]

plane strain (3-14)

\[ E = \text{Elastic modulus, } \nu = \text{Poisson's ratio} \]

3.2.1 Boundary conditions

Two classes of boundary conditions called essential and natural boundary conditions are identified in solid mechanics.

The essential boundary conditions are also called geometric boundary conditions because in structural mechanics the essential boundary conditions correspond to prescribed displacements and rotations.

The second class of boundary conditions, namely, the natural boundary conditions, are also called force boundary conditions correspond to prescribed boundary forces and moments.

\[ t_x = \sigma_{xx} n_x + \sigma_{xy} n_y = \tilde{f}_x \quad \text{Natural} \]
\[ t_y = \sigma_{yx} n_x + \sigma_{yy} n_y = \tilde{f}_y \]

\[ u = \tilde{u}, \quad v = \tilde{v} \quad \text{Essential} \] (3-15)

where \((n_x, n_y)\) are the components (or direction cosines) of the unit normal vector \(\tilde{n}\) on the boundaries of the solid domain.

The boundary stress components (or tractions) can also be expressed in terms of the displacements:

\[ E = \text{Elastic modulus, } \nu = \text{Poisson's ratio} \]
Chapter 3 Mathematical model

3.3 Basic equations of fluid flow:

In obtaining the basic equations of the fluid motion, the following philosophy is always followed:

A. choose the appropriate fundamental physical principals from the law of physics such as:
   a. Mass is conserved which lead to continuity equation
   b. Newton’s second law which lead to momentum balance
   c. Energy is conserved which lead to energy balance

B. Apply these physical principals to a suitable model of the flow.

From this application, extract the mathematical equations which embody such physical principals.

Fluid governing equations are obtained from combining the laws of mass, momentum, and energy with constitutive equations describing the behaviour of each class of fluids.

3.3.1 Continuity equation

The continuity equation is the expression of the law of conservation of mass. This equation is written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{v} = 0$$

(3-18)

For incompressible fluid, first term in equation (3-18) will be omitted.

3.3.2 Equation of motion
3.3.2.1 Fluid flow in a free domain:

The equation of motion is based on the law of conservation of momentum. This equation is written as:

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \nabla \mathbf{v} = \nabla \sigma + \rho \mathbf{g}$$  \hspace{1cm} (3-19)

where $\rho$ is fluid density, $\mathbf{v}$ is velocity, $\sigma$ is the Cauchy stress tensor and $\mathbf{g}$ is the body force per unit volume of fluid. For the fluids with very low Reynolds numbers (highly viscous fluids, e.g. polymers), the convection term (i.e. $\mathbf{v} \nabla \mathbf{v}$) in equation (3-19) is usually small and can be neglected, and combining this situation with Newtonian constitutive equation leads to Stokes governing equation.

The Cauchy stress is given as:

$$\sigma = -p \delta + \tau$$  \hspace{1cm} (3-20)

where $p$ is static pressure, $\delta$ is unit second-order tensor (kronecker delta) and $\tau$ is the extra stress tensor. The equation of motion is hence written as:

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \nabla \mathbf{v} = -\nabla p \delta + \nabla \tau + \rho \mathbf{g}$$  \hspace{1cm} (3-21)

3.3.2.2 Fluid flow in a Porous medium:

In a porous structure, the global transport of momentum by shear stresses in the fluid is negligible as the pore walls impede momentum transport to fluid outside the individual pores. A detailed description, down to the resolution of every pore, is not practical in most models, so homogenization of the porous and fluid media into one single medium is a common approach. Darcy's law is based upon this approach and describe flow in porous media where the pressure gradient is the only driving force. Darcy's law states that the velocity vector is determined by the pressure gradient, the fluid viscosity and the structure of the porous media.

$$u = -\frac{k}{\eta} \nabla p$$  \hspace{1cm} (3-22)
where \( k \) denotes the permeability of the porous media, \( \eta \) the fluid viscosity, \( p \) the pressure and \( u \) the velocity vector.

The Brinkman equations describe flow in porous media where momentum transport by shear stresses in the fluid is of importance. The model extends Darcy’s law to include a term that accounts for the viscous transport, in the momentum balance, and introduces velocities in the spatial directions as dependent variables.

The flow field is determined by the solution of the momentum balance equations in \( x \), \( y \), and \( z \) directions:

\[
\rho \frac{\partial u}{\partial t} + \nabla \cdot \left[ -\eta (\nabla u + (\nabla u)^T) + pI \right] = -\frac{\eta}{\kappa} u
\]  

(3-23)

### 3.3.3 Boundary conditions for the fluid

**Inlet conditions**

Typically velocity components along the inlet are given as essential (also called Dirichlet)-typed boundary conditions. For example, for a flow entering the domain shown in Figure 3.1 they can be given as following forms on the inlet boundary (left side of the domain):

\[
\begin{align*}
\nu_y &= 0 \\
\nu_x &= \nu_x(y)
\end{align*}
\]  

(3-24)

![Figure 3-1: boundary lines in a flow domain](image)
Solid walls
On no-slip walls zero velocity components can be readily imposed as the required boundary conditions.

Exit conditions
Typically the exit velocity in the flow domain is unknown and hence the prescription of Drichlet-type boundary conditions at the outlet is not possible. However, at the outlet of sufficiently long domains fully developed flow conditions may be imposed. In the flow domains that are not considered to be long enough to impose developed flow conditions, stress-free conditions at the domain outlet may be used. In this case, both shear and normal components of the surface forces at the exit are set to zero. This is satisfied by setting the boundary integral along the exit line to zero.

Papanastasiou et al. [84] suggested that in order to generate realistic solution for Navier-Stokes equations the exit conditions should be kept free (no outlet conditions should be imposed).

Line of symmetry
The normal component of velocity and tangential component of surface force are set to zero along a line of symmetry. For the domain shown in Figure 3.1 these are expressed as

\[
\begin{align*}
    v_y &= 0 \\
    \sigma_{xy} &= 0
\end{align*}
\]  

(3-25)

Imposing of the first condition is identical to the procedure used for prescribing inlet velocity components and second condition is simply satisfied by setting the boundary line integral in the discretized equation of motion to zero.

3.4 Mathematical model for the deformation of porous medium and fluid flow in porous medium
To derive the governing equations for porous media, a system consisting of an incompressible fluid and porous structure has been considered. The unknown field functions are liquid pressure $p$ and solid displacement $u$.

The deformation process is modelled by the system

$$\nabla.(\sigma - pI) + \rho g = 0 \quad \text{in } \Omega$$

$$\sigma - Ce(u) = 0 \quad \text{in } \Omega$$

where $\sigma$ denotes the effective stress, and the momentum balance equation is modified such that it incorporates stresses and forces connected to the fluid pressure. Also, $C$ is the elasticity tensor representing the dependence of strain and stress for a linear elastic material law.

Assuming the isotropic problem being considered, the stress tensor $\sigma$ and strain tensor $\varepsilon$ are introduced in a vector form as

$$\sigma = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{zx})^T$$

$$\varepsilon = (\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{yz}, \varepsilon_{zx})^T$$

for geometrically linear elasticity, the strain is defined as

$$\varepsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$$

which can be written in the form

$$\varepsilon(u) = \ell u$$

with the definition of the gradient operator and displacement

$$\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$$

$$u = (u_x, u_y, u_z)^T$$

and the differential operator
fluid flow in deformable porous media described by the following mass and momentum balance equations,

\[ \nabla \cdot \mathbf{w} + \nabla \cdot \frac{\partial \mathbf{u}}{\partial t} = 0 \quad \text{in } \Omega \quad (3-32) \]

\[ \mathbf{w} + \frac{k}{\mu} (\nabla p - \rho g) = 0 \quad \text{in } \Omega \quad (3-33) \]

In consolidation theory, the fluid mass balance equation (3-32) has an extra term due to deformation process. The second equation (3-33) is denoted as the Darcy's law. Here, \( \mathbf{w} \) denotes the volumetric flux of the fluid and \( p \) is the fluid phase pressure. \( k \) denotes the permeability tensor, \( \mu \) is the fluid viscosity, and \( \rho \) is the density of the porous medium. Hereby it is assumed that solid grains themselves are incompressible.

### 3.4.1 Porous flow boundary conditions

The flow conditions that can be applied to the boundary of a fluid-saturated porous medium depend on the specific model used to describe the problem. For the Brinkman equation, the admissible boundary conditions are the same as those given for the Stokes equation.

For the Darcy's model, either the velocities (outflow/inflow) or the force (pressure) normal to the boundary may be imposed. This model neither allows the imposition of a tangential velocity (e.g., no-slip walls are not admissible) nor the specification of viscous forces on the boundary.
4.1 General outline

A finite element program consists of three basic parts

1. pre-processor
2. processor
3. postprocessor

In the pre-processor part of the program, the input data of the problem are read in and/or generated. This includes the geometry (e.g., length of the domain and boundary conditions), the data of the problem (e.g., coefficients in the differential equation), finite element mesh information (e.g., element type, number of elements, element length, coordinates of the nodes, the connectivity matrix), and indicators for various options (e.g., type of field problem analyzed, static analysis, eigenvalue analysis, transient analysis, and degree of interpolation).

In the processor part, all steps in the finite element method are performed. These include the following:

2. Assembly of element equations.
3. Imposition of the boundary conditions.
4. Solution of the algebraic equations for the nodal values of the primary variables.

In the postprocessor part of the program, the solution is computed by interpolation at points others than nodes, and secondary variables that are derivable from the solution are also computed.
The processor, where typically most of the computing time is spent, can consist of several subroutines, each having a special purpose (e.g., a subroutine for the calculation of element matrices, a subroutine for imposition of the boundary conditions, and a subroutine for the solution of the equations). The degree of sophistication and complexity of a finite element program depends on the general class of problem being programmed and the generality of the data in the equations.

4.2 The finite element method

The finite element method is a numerical procedure for solving the differential equations of physics and engineering. The method has its birth in the aerospace industry in the early 1950s and was presented in the publication by Turner, Clough, Martin, and Topp [85]. This publication stimulated other researchers and resulted in several technical articles that discussed the application of the method to structural and solid mechanics.

The connecting of the finite element method with a minimization procedure quickly led to its use in other engineering areas. The method was applied to problems governed by the Laplace or the Poisson equations because these equations are closely related to the minimization of a functional.

The range of applications for the finite element method was enlarged when the investigators (Zienkiewicz, [86]) showed that the element equations related to structural mechanics, heat transfer, and fluid mechanics could also be derived by using either a weighted residual procedure such as Galerkin's method or the Least-Squares approach. This was a very important contribution to the theory because it allowed the finite element method to be applied to any differential equation.

The finite element method has advanced from a specific numerical procedure for solving structural problems to a more general numerical procedure for solving a system of differential equations.

Several advantageous properties of the finite element method have contributed to its extensive use. Some of the main ones include:
1- The material properties in adjacent elements do not have to be the same. This allows the method to be applied to bodies composed of several materials.

2- Irregularly shaped boundaries can be approximated using elements with straight sides or matched exactly using elements with curved boundaries. The method, therefore, is not limited to nice shapes with easily defined boundaries.

3- The size of elements can be varied. This property allows the element grids to be expanded or refined as the need arises.

4- Boundary conditions such as discontinuous surface loadings present no difficulties for the method. Mixed boundary conditions can be easily handled.

5- The above properties can be incorporated into one general computer program for a particular subject matter area. For example, a general computer program for axisymmetric heat transfer is capable of solving any problem of this type that may arise.

The primary disadvantage of the finite element method is the need for computer programs and computer facilities. The computations involved in the finite element method are too numerous for hand calculations even when solving very small problem. The digital computer is necessary, and computers with large memories are needed to solve large complicated problems.

4.3 Finite element models for incompressible flows

In order to deal with the incompressibility constraint and satisfying the stability condition known as Ladyzhenskaya-Babuska-Brezzi (LBB) conditions, two different finite element schemes have been considered. The first is a natural and direct formulation in which the three equations in $u$, $v$ and $p$ are used in their original form. This formulation is known as the velocity-pressure formulation. The other is based on
the interpolation that the continuity equation is an additional relation among the velocity components and this constraint is satisfied in a least-squares sense. This particular method of including the constraint in the formulation is known as the penalty function method.

4.3.1 Working equations for the Fluid flow

4.3.1.1 Stokes flow with penalty scheme

To derive the working equations for the Stokes flow, the starting point is the governing equations which have been described in chapter 3. Applying the weighted residual Galerkin method, the equations are multiplied by the weight functions and then integrated over the whole domain.

\[
\nabla \left\{ \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y} \right\} - 2 \frac{\partial}{\partial x} \left\{ \frac{\partial}{\partial x} \right\} - \frac{\partial}{\partial y} \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \right\} = 0
\]

(4-14)

\[
\nabla \left\{ \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y} \right\} - 2 \frac{\partial}{\partial x} \left\{ \frac{\partial}{\partial x} \right\} - \frac{\partial}{\partial y} \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \right\} = 0
\]

Also the integration by part has been used to trade the equality between the weight function and the dependent variables. As the result, the following set of equations have been derived:

\[
[K^{11}] \{u\} + [K^{12}] \{v\} = \{F^1\}
\]

(4-15)

\[
[K^{21}] \{u\} + [K^{22}] \{v\} = \{F^2\}
\]

where
Chapter 4 Numerical scheme

\[ K_{ij}^{11} = \int_{\Gamma} \left( \lambda + 2\eta \right) \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \, dx \, dy \]

\[ K_{ij}^{12} = \int_{\Gamma} \left( \lambda \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \right) \, dx \, dy \]

\[ K_{ij}^{21} = \int_{\Gamma} \eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \, dx \, dy \]

\[ K_{ij}^{22} = \int_{\Gamma} \left[ \eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + (\lambda + 2\eta) \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \right] \, dx \, dy \]

\[ F_1 = \int_{\Gamma} N_i \left[ \lambda \left( \frac{\partial u^e_x}{\partial x} + \frac{\partial u^e_y}{\partial y} \right) + 2\eta \frac{\partial u^e_x}{\partial y} \right] n_x + \eta \left( \frac{\partial u^e_y}{\partial y} + \frac{\partial u^e_x}{\partial x} \right) n_y \right] \, d\Gamma_e \]

\[ F_2 = \int_{\Gamma} N_i \left[ \lambda \left( \frac{\partial u^e_x}{\partial x} + \frac{\partial u^e_y}{\partial y} \right) + 2\eta \frac{\partial u^e_x}{\partial y} \right] n_x + \eta \left( \frac{\partial u^e_y}{\partial y} + \frac{\partial u^e_x}{\partial x} \right) n_y \right] \, d\Gamma_e \]

Full description of the working equations of the fluid using perturb continuity method for both free flow (Stokes equation) and porous flow (Darcy equation) can be found in the literature [87].

4.3.1.2 Working equations for free flow region with Taylor-Hood elements (UVP scheme)

The final working equations for free flow (Stokes equation) in transient state are as follows. Theta method has been used to in order to derive the transient form of equations.

\[
\begin{bmatrix}
A_{i1}^{11} & A_{i1}^{12} & A_{i1}^{13} \\
A_{i2}^{11} & A_{i2}^{12} & A_{i2}^{13} \\
A_{i3}^{11} & A_{i3}^{12} & A_{i3}^{13}
\end{bmatrix}
\begin{bmatrix}
U_j \\
V_j \\
P_j
\end{bmatrix}
^{n+1} =
\begin{bmatrix}
K_{i1}^{11} & K_{i1}^{12} & K_{i1}^{13} \\
K_{i2}^{11} & K_{i2}^{12} & K_{i2}^{13} \\
K_{i3}^{11} & K_{i3}^{12} & K_{i3}^{13}
\end{bmatrix}
\begin{bmatrix}
U_j \\
V_j \\
P_j
\end{bmatrix}
^{n} +
\begin{bmatrix}
R_1^j \\
R_2^j \\
R_3^j
\end{bmatrix}
^{n+1}
\]
\[ A^{11}_{ij} = \int_{\Omega} \theta \Delta t \left( 2\eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) dx dy \]

\[ A^{12}_{ij} = \int_{\Omega} \theta \Delta t \left( \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \right) dx dy \]

\[ A^{13}_{ij} = -\int_{\Omega} \theta \Delta t \left( M_j \frac{\partial N_i}{\partial x} \right) dx dy \]

\[ A^{21}_{ij} = \int_{\Omega} \theta \Delta t \left( \eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \right) dx dy \]

\[ A^{22}_{ij} = \int_{\Omega} \theta \Delta t \left( \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + 2\eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} \right) dx dy \]

\[ A^{23}_{ij} = -\int_{\Omega} \theta \Delta t \left( M_j \frac{\partial N_i}{\partial y} \right) dx dy \]

\[ A^{31}_{ij} = -\int_{\Omega} \theta \Delta t \left( M_i \frac{\partial N_j}{\partial x} \right) dx dy \]

\[ A^{32}_{ij} = -\int_{\Omega} \theta \Delta t \left( M_i \frac{\partial N_j}{\partial y} \right) dx dy \]

\[ A^{33}_{ij} = 0 \]

\[ K^{11}_{ij} = \int_{\Omega} \left[ (\theta - 1) \Delta t \left( 2\eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) \right] dx dy \]

\[ K^{12}_{ij} = \int_{\Omega} \left[ (\theta - 1) \Delta t \left( \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \right) \right] dx dy \]
4.4 Working equations for the Solid phase

To derive the working equations for the solid elastic phase, the starting point is the governing equations which have been described in chapter 3.

\begin{align*}
-\frac{\partial}{\partial x} (C_{11} \frac{\partial u}{\partial x} + C_{12} \frac{\partial v}{\partial y}) - \frac{\partial}{\partial y} \left( C_{33} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right) &= 0 \\
-\frac{\partial}{\partial y} (C_{12} \frac{\partial u}{\partial x} + C_{22} \frac{\partial v}{\partial y}) - \frac{\partial}{\partial x} \left( C_{33} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right) &= 0 
\end{align*}

(4.19)

Applying the weighted residual Galerkin method, the equations are multiplied by the weight functions and then integrated over the whole domain. Also the integration by
part has been used to trade the equality between the weight function and the dependent variables. As the result, the following equations have been derived:

\[
0 = \int_\Omega \left( C_{11} \frac{\partial u}{\partial x} + C_{12} \frac{\partial v}{\partial y} + C_{66} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right) dxdy - \frac{1}{r} \int_{\Gamma} w_1 [(C_{11} \frac{\partial u}{\partial x} + C_{12} \frac{\partial v}{\partial y}) n_x + C_{66} (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) n_y] ds
\]

(4-19)

Appointing the values of weighted functions equal to interpolation function results in the following set of equations for the plane elasticity problems:

\[
[K^{11}] \{u\} + [K^{12}] \{v\} = \{F^1\}
\]

(4-20)

\[
[K^{21}] \{u\} + [K^{22}] \{v\} = \{F^2\}
\]

where

\[
K_{ij}^{11} = \int_\Omega \left( c_{11} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + c_{66} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) dxdy
\]

\[
K_{ij}^{12} = K_{ji}^{21} = \int_\Omega \left( c_{12} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} + c_{66} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \right) dxdy
\]

(4-21)

\[
K_{ij}^{22} = \int_\Omega \left( c_{66} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + c_{12} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) dxdy
\]
\[ F^1_i = \int_{\Omega} N_i f \, dx \, dy + \oint_{\Gamma} N_i t \, ds \]  
\[ F^1_i = \int_{\Omega} N_i f \, dx \, dy + \oint_{\Gamma} N_i t \, ds \]  
\[ t_x = (c_{11} \frac{\partial u}{\partial x} + c_{12} \frac{\partial v}{\partial y})n_x + c_{33} (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})n_y \]  
\[ t_y = c_{33} (\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})n_x + (c_{12} \frac{\partial u}{\partial x} + c_{22} \frac{\partial v}{\partial y})n_y \]  
\[ c_{11} = c_{22} = \frac{E}{1-\nu^2}, \quad c_{12} = \frac{\nu E}{1-\nu^2}, \quad c_{33} = \frac{E}{2(1+\nu)} \text{ plane stress (4-24)} \]  
\[ c_{11} = c_{22} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}, \quad c_{12} = \frac{\nu E}{(1+\nu)(1-2\nu)}, \quad c_{33} = \frac{E}{2(1+\nu)} \text{ plane strain (4-25)} \]  

Similarity in the resultant fluid (4-16,4-17) and solid (4-21,4-22) equations provides a means for representing a unique set of equations for both regions. This approach has the flexibility to switch the model from fluid analysis to solid deformation. This results in a significant reduction in computational cost. However, this procedure depends on considering the following relationships which relate the penalty parameter in the fluid equation to Young’s modulus and Poisson’s ratio.

For plane strain \[ \lambda = \frac{2\nu E}{(1-2\nu)} \]  
For plane stress \[ \lambda = \frac{2E\nu}{1-\nu} \]
4.5 UVP Formulation of fluid flow and deformation in porous medium

For the UVP formulation of the consolidation problem the system (4-28), (4-29) and (4-30) is reduced to two second order equations. This is achieved by plugging in the constitutive relationships of fluid into mass and linear momentum, equations respectively. Primary variables of this formulation are fluid pressure and solid displacement. Secondary variables are fluid flux vector and stress tensor.

\[ \nabla.(\sigma - pI) + \rho g = 0 \quad \text{in } \Omega \]  
(4-28)

\[ \sigma - C \epsilon(u) = 0 \quad \text{in } \Omega \]

\[ \nabla.w + \nabla.\frac{\partial u}{\partial t} = 0 \quad \text{in } \Omega \]  
(4-29)

\[ w + \frac{k}{\mu}(\nabla.p - \rho g) = 0 \quad \text{in } \Omega \]  
(4-30)

The combination of (4-29) and (4-30) leads to the equation

\[ - \nabla.\frac{k}{\mu}(\nabla.p - \rho g) + \nabla.\frac{\partial u}{\partial t} = 0 \]  
(4-31)

for the fluid mass balance of the porous medium. The porous medium momentum conservation is described in terms of the displacement field [equation (4-32)]

\[ \nabla.(C(\epsilon) - pI) + \rho g = 0 \]  
(4-32)

The UVP formulation consists of the two differential equations of second order for p and u.
4.5.1 Finite element discretization of the deformation and fluid flow in porous medium

The method of weighted residuals is applied to derive the weak formulation of the porous medium mass conservation equation. In order to eliminate the second order derivatives Gauss-Green integral theorem has been used. This leads to

\[
\int_\Omega \omega (\nabla \frac{\partial u}{\partial t}) d\Omega + \int_\Omega \nabla \omega \cdot (\frac{k}{\mu} (\nabla p - \rho g)) d\Omega = -\int_{\partial \Omega} \omega W \cdot n d\Gamma
\]  

(4-33)

which needs to hold for appropriate sets of weighting functions \( \omega \). Here, \( W \cdot n \) is the normal vector of fluid mass flux term. All unknown functions are approximated by trial solutions based on nodal values and interpolation functions

\[
p = \sum_{k=1}^{n_p} N^k_p \tilde{p}_k
\]

(4-34)

where \( \tilde{p}_k \) is the solution for fluid pressure in finite element space, or nodal values, and \( N^k_p \) are shape functions. For the determination of both, fluid pressure \( p \) and solid displacement \( u \), the following system of algebraic equations can be derived as the result of spatial discretization,

\[
K^*_p \tilde{p} + C_u^* \frac{d\tilde{u}}{dt} = f^*_p
\]

(4-35)

where \( f^*_p \) is the right-hand side vector associated with the integration of body forces and the Dirichlet boundary conditions.

Time discretization using first order finite difference scheme yields the following scheme:

\[
K^*_{pp} \tilde{p}^{i+1} + \frac{C_u^*}{\Delta t} \tilde{u}^{i+1} = \frac{C_u^*}{\Delta t} \tilde{u}^i + f^*_p
\]

(4-36)

where exponents \( i \) and \( i+1 \) denote old new time levels, respectively.

The weak form of the stress equilibrium equation must be fulfilled throughout the load history, i.e.,
for the virtual velocity field \( \delta v \in \mathbb{R}^m, m=2,3 \) that satisfies \( \delta v = 0 \) on \( \partial \Omega_u \) if isotropic mechanical properties are assumed for this medium.

In the finite element space, the displacement \( u \) can be interpolated by

\[
\mathbf{u} = \sum_{k=1}^{n_u} N_u^k \hat{\mathbf{u}}_k
\]

(4-38)

where \( \hat{\mathbf{u}}_k \in \mathbb{R}^m \) are exactly the components of \( \mathbf{u} \) and \( N_u^k \) is the shape function for displacement. Using the differential operator defined previously the approximation can be put as

\[
\mathbf{\varepsilon} = \ell N_u \hat{\mathbf{u}} = B \hat{\mathbf{u}}
\]

(4-39)

based on the usual Galerkin procedure, the following finite element formulation can be derived for the weak form of the momentum balance equation

\[
K_{u \mathbf{p}}^* \mathbf{p}^* + K_{u u}^* \mathbf{u}^* = f_u^*
\]

(4-40)

equations (4-36) and (4-40) build a set of coupled linear equations to be solved for the primary variables liquid pressure \( p \) and solid displacement \( u \) of the UVP formulation of consolidation problem. The resulting equation system can be compactly written in following form:

\[
\begin{bmatrix}
K_{pp} & \frac{1}{\Delta t} C_u^* \\
K_{u p}^* & K_{u u}^*
\end{bmatrix}
\begin{bmatrix}
\mathbf{p}^{i+1} \\
\mathbf{u}^{i+1}
\end{bmatrix} = \begin{bmatrix}
f_p^* + \frac{1}{\Delta t} C_u^* \mathbf{u}^i \\
f_u^*
\end{bmatrix}
\]

(4-41)

\[
K_{pp} = \int_\Omega \nabla N_p \frac{k}{\mu} \nabla N_p d\Omega
\]

fluid conductance matrix

(4-42)

\[
C_u^* = \int_\Omega N_p (m^T \ell) N_u d\Omega = \int_\Omega N_p m^T B d\Omega
\]

dilatation coupling matrix

(4-43)
Chapter 4 Numerical scheme

\[ f_p^* = \int_{\Omega} \nabla N_p \left( \frac{k}{\mu} \rho g \right) d\Omega - \int_{\Gamma} N_p \bar{\sigma} d\Gamma \quad \text{fluid pressure load vector} \quad (4-44) \]

\[ K_{wp}^* = -(C_u^*)^T \quad \text{fluid pressure coupling matrix} \quad (4-45) \]

\[ K_{ua}^* = \int_{\Omega} B^T C B d\Omega \quad \text{stiffness matrix} \quad (4-46) \]

\[ f_u^* = \int_{\Omega} N_u^T \rho g d\Omega + \int_{\Gamma} N_u \bar{\sigma} d\Gamma \quad \text{load vector} \quad (4-47) \]

where \( \text{m} \) is a mapping vector given by

\[ m = (1,1,0,0,0)^T \quad (4-48) \]

for 3D problems,

\[ m = (1,1,1)^T \quad (4-49) \]

for plane strain problems and

\[ m = (1,1,0)^T \quad (4-50) \]

for plane stress problems.

Matrix \( C_u^* \) is geometry dependent only. It can be computed once and stored for successive computations.

4.5.2 Working equations of fluid flow and solid deformation in porous medium using the Taylor-Hood elements (UVP scheme)

The procedure to develop transient form of the governing equation in order to be implemented in the finite element code is the same as the ones in section 4.7. Starting from the governing equation and following the steps in section 4.7.1 results in following sets of equations:
\[
\begin{bmatrix}
A_{ij}^{11} & A_{ij}^{12} & A_{ij}^{13} \\
A_{ij}^{21} & A_{ij}^{22} & A_{ij}^{23} \\
A_{ij}^{31} & A_{ij}^{32} & A_{ij}^{33}
\end{bmatrix}
\begin{bmatrix}
U_j^{n+1} \\
V_j^{n+1} \\
P_j^{n+1}
\end{bmatrix}
= 
\begin{bmatrix}
K_{ij}^{11} & K_{ij}^{12} & K_{ij}^{13} \\
K_{ij}^{21} & K_{ij}^{22} & K_{ij}^{23} \\
K_{ij}^{31} & K_{ij}^{32} & K_{ij}^{33}
\end{bmatrix}
\begin{bmatrix}
U_j^n \\
V_j^n \\
P_j^n
\end{bmatrix}
+ 
\begin{bmatrix}
R_j^1 \\
R_j^2 \\
R_j^3
\end{bmatrix}
\] (4-51)

\[A_{ij}^{11} = \int_\Omega [\theta (C_{i1} \frac{\partial N_j}{\partial x} + C_{33} \frac{\partial N_{i1}}{\partial y} + \frac{\partial N_{i1}}{\partial x} \frac{\partial N_{i1}}{\partial y})] \, dx \, dy\]

\[A_{ij}^{12} = \int_\Omega [\theta (C_{36} \frac{\partial N_{i1}}{\partial y} + C_{33} \frac{\partial N_{i1}}{\partial x} \frac{\partial N_{i1}}{\partial y})] \, dx \, dy\]

\[A_{ij}^{13} = -\int_\Omega [\theta (M_{ij})] \, dx \, dy\]

\[A_{ij}^{21} = \int_\Omega [\theta (C_{12} \frac{\partial N_{i1}}{\partial x} + C_{33} \frac{\partial N_{i1}}{\partial y})] \, dx \, dy\]

\[A_{ij}^{22} = \int_\Omega [\theta (C_{22} \frac{\partial N_{i1}}{\partial y} + C_{33} \frac{\partial N_{i1}}{\partial x})] \, dx \, dy\]

\[A_{ij}^{23} = -\int_\Omega [\theta (M_{ij})] \, dx \, dy\]

\[A_{ij}^{31} = \int_\Omega [\theta (M_{ij})] \, dx \, dy\]

\[A_{ij}^{32} = \int_\Omega [\theta (M_{ij})] \, dx \, dy\]

\[A_{ij}^{33} = \int_\Omega [\theta\Delta t \frac{\eta}{k} (\frac{\partial N_{i1}}{\partial y} + \frac{\partial N_{i1}}{\partial x}) + \frac{\partial N_{i1}}{\partial x}] \, dx \, dy\]

\[K_{ij}^{11} = \int_\Omega [(\theta - 1) (C_{11} \frac{\partial N_j}{\partial x} + C_{36} \frac{\partial N_{i1}}{\partial y})] \, dx \, dy\]
\[ K_{ij}^{12} = \int_{\Omega} \left[ (\theta - 1) \left( C_{33} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} + C_{12} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \right) \right] \, dx \, dy \]

\[ K_{ij}^{13} = \int_{\Omega} \left[ (1 - \theta) M_i \frac{\partial N_j}{\partial x} \right] \, dx \, dy \]

\[ K_{ij}^{21} = \int_{\Omega} \left[ (\theta - 1) \left( C_{12} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + C_{66} \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} \right) \right] \, dx \, dy \]

\[ K_{ij}^{22} = \int_{\Omega} \left[ (1 - \theta) M_i \frac{\partial N_j}{\partial y} \right] \, dx \, dy \]

\[ K_{ij}^{23} = \int_{\Omega} \left[ (1 - \theta) M_i \frac{\partial N_j}{\partial y} \right] \, dx \, dy \]

\[ K_{ij}^{31} = \int_{\Omega} \left[ (M_i \frac{\partial N_j}{\partial x}) \right] \, dx \, dy \]

\[ K_{ij}^{32} = \int_{\Omega} \left[ (M_i \frac{\partial N_j}{\partial y}) \right] \, dx \, dy \]

\[ K_{ij}^{33} = \int_{\Omega} \left[ (\theta - 1) \Delta t \frac{\eta}{k} \left( \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} \right) \right] \, dx \, dy \]

### 4.7 Stress computation in fluid domain

The results of interest from a flow analysis generally include fluid velocities, forces, and flow patterns. Many of these items are directly available from the finite element results in terms of nodal point quantities; other quantities of interest may be derived from these primary variables. The computation of viscous stress fields for the fluid flow follow directly from the finite element approximations of these variables.
For a planar two-dimensional geometry, the components of the stress tensor \((\sigma_{xx}, \sigma_{yy}, \sigma_{xy})\) are known in terms of pressure \(P\) and velocity components \(u\) and \(v\).

\[
\begin{align*}
\sigma_{xx} &= -p + 2\eta \frac{\partial u}{\partial x} \\
\sigma_{yy} &= -p + 2\eta \frac{\partial v}{\partial y} \\
\sigma_{xy} &= \eta \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \quad (4-63)
\end{align*}
\]

Since the stresses depend on velocity gradients they are discontinuous between elements. The derivative quantities are normally evaluated at Gauss integration points in the interior of elements. These points have optimal accuracy for the shape function derivatives and correspond to the least squares approximation for the derivative. The stresses computed at interior integration points can be extrapolated to the nodes by a simple linear extrapolation procedure, and they may be appropriately averaged between adjacent elements to produce continuous stress fields.
4.8 Solution strategy and developed algorithm for fluid –solid interaction problem

Two methodologies have been applied in the present work for the solution of fluid-solid problems. In the first method, the equations of solid and fluid are connected to each other at the interface and solved simultaneously with a single code. The following flowchart explains the procedure in details. Nassehi et.al [88] proposed a method to connect different fluids working equations when simulating free-porous flow regimes. This technique is explained in section 5.12 and used in the present work for the interaction of fluid and solid.

In the second method the fluid and solid parts are solved in a separate manner. The fluid flow is solved first and the resultant forces from the fluid on the interfacial nodes are calculated. Then, the resultant forces are transferred to the solid and used as boundary conditions for the structural computations. As the solid is considered to be porous, the flow equation in the solid (Darcy equation) have to be solved in connection with the free flow (Stokes equation).

In order to solve the fluid flow equations the following steps are followed.

The members of the sub-matrices and sub-vectors of the finite element working equations are calculated by the use of iso-parametric mapping and a gauss quadrature method. The resulting algebraic equations are assembled into a global matrix and after imposing the appropriate set of the first type boundary conditions, solved by a frontal solution algorithm. The dependency of the viscosity on the velocity gradient, make the set of assembled equations non-linear. Therefore, an iterative procedure based on Picard’s iteration method has been adopted. The following steps summarized the solution strategy based on the mentioned technique.

1. The entire domain of interest is first discretized into a mesh of finite element.
2. Using a set of initial values (zero if it is the first iteration) for the components of the velocity vector, the coefficient matrices of the flow working equations are computed.

3. The assembled working equations are then solved to obtain velocity and displacement fields.

4. Using the set of auxiliary equations viscosity is updated using the power-law model;

5. Step 3 is iterated until convergence is reached. Convergence is checked using a calculated ratio of the Euclidean norm between successive iterations to the norm. The converged solution should satisfy

\[
\frac{\sum_{i=1}^{N} (X_{i}^{r+1} - X_{i})^2}{\sqrt{\sum_{i=1}^{N} X_{i}^{r+1}^2}} \leq \varepsilon
\]

where \( i \) is the number of iteration cycle, \( N \) is the total number of degree of freedom and \( \varepsilon \) is a pre-selected convergence tolerance value.
Chapter 4

No

Element on the interface?

Yes

Evaluate the components of stiffness matrix inserting the fluid flow components

Is the node on the interface?

Yes

Replace the fluid flow terms corresponding to the interface nodes by solid deformation terms

No

Evaluate the components of stiffness matrix inserting the fluid flow components

If \( n_e > m \)

Yes

Evaluate the components of stiffness matrix inserting the solid deformation components

No

Evaluate the components of stiffness matrix inserting the fluid flow components

Assemble the stiffness matrices and load vectors of all elements into final mega matrix

No

Are all of the elements assembled?

Yes

Input the B.C and Solve the final global stiffness matrix

Figure 4-1 the modeling strategy

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4.8.1 Linking of the working equations of flow and solid phase

To couple the different governing equations of solid and fluid phases, the solid phase equations are imposed as the boundary condition for the fluid equations at the interface between the phases. This imposition circumvents the difficulty of matching the unequal line integrals which arise during the discretization of governing equations of two phases. In the stiffness matrix of fluid elements, terms representing the fluid-solid interface are replaced by terms resulting from the discretization of solid displacement equations. This procedure is illustrated in Figure 5.6.

Figure 4-2 schematic representation of linking phases in this work

Figure 4-2 shows two different elements X and Y connected in series. Element X is in the fluid region connected to element Y in the solid region. The boundary AB of the element X coincides with boundary CD of element Y at the interface. In real sense, both these boundaries AB and CD coincide at the interface.

I₁, J₁, K₁ are the nodes of flow element X on the interface AB-CD, whereas I₂, J₂, K₂ are the nodes of solid element Y on the same interface. In the final matrix assembly, the terms of the stiffness matrix of fluid element X are replaced by the terms of corresponding nodes I₂, J₂, K₂ from the stiffness matrix of the neighbouring element Y which is in the solid region. Therefore, instead of specifying artificial boundary condition on the interface, this is the direct linking of two different regions.

In case of complex geometry of the domain, distorted elements in the computational mesh need to be used. Therefore, the distorted working equations are transformed into local natural coordinate system using isoparametric mapping. The integrals in the elemental stiffness equations are hence calculated using Gauss-Legendre Quadrature.
After the evaluation of the members of the elemental stiffness matrices, they are assembled over common nodes in the computational grid to obtain a system of algebraic equations. After insertion of the boundary conditions, this system becomes determinate and can be solved using non-symmetric frontal solver. Details of the above operations can be found in the standard finite element literature [89].
Chapter 4

Solve fluid flow equations using updated solid boundaries.

Use the obtained solution to calculate the stresses on the surface of the leaflet.

Apply the calculated stress as the boundary condition and find elastic deformation and displacement.

Check the physical accuracy of the simulated fluid/solid deformation fields.

Update the domain geometry.

Write the result into the initial conditions file.

End of simulation

Prepare the output file

Stop

Converged

No

Yes

Figure 4-3 the modeling strategy’s flowchart
Results and discussions

The results in this thesis were obtained using a Pentium 4 processor on a personal desktop computer. The pre-processing and part of post-processing were done using Geostar software supplied by Structural Research & Analysis Corp and TECPLOT software supplied by AMTEC Corp. USA, Inc. was also used for post-processing. Geostar is an interactive 2D/3D geometric modeller providing pre- and post-processors analyses. A FORTRAN code has been developed to carry out the computations and simulations. In addition, the commercial modelling software COMSOL has been used in this study in conjunction with the developed code in FORTRAN.

5.1 Presentation of results

The resultant velocity vectors are plotted in colour using the TECPLOT software. The software plots the vectors by magnitude on a colour scale. A sample scale is shown in Figure 5-1. The scale shows the increase of velocities from blue to red region which means that low velocities are in the blue category whilst high ones are in red region of the scale. Some velocity results are presented in contour form using Geostar. All the velocities are in the units of meter per second (ms⁻¹) unless stated otherwise.

![Figure 5-1 A sample velocity scale](image-url)
The directions for the vectors can be assessed in accordance with the orientation of axes represented in Figure 5-2.

![Figure 5-2 velocity vector representation](image)

The coloured pressure contours were generated using Geostar. Figure 5-3 shows a sample colour pressure contour. Similar to velocity, the lowest pressure value is in the blue region whilst the highest value is in the deep red region. All the pressure units are in Pascal (Pa) unless stated otherwise.

![Figure 5-3 A sample pressure contour scale](image)

Based on the explained methods in the previous chapters, some benchmark Fluid-solid and fluid-porous solid interaction problems are solved.

Section 5.2 is devoted to fluid flow simulation, followed by sections 5.3 and 5.4 with the solution of fluid-solid and fluid-porous solid interaction systems. The solved examples in each section are typical examples of physical phenomena occurring in the chemical engineering field including reactor design and filtration.
5.2 Fluid flow

Two problems in the chemical engineering field have been solved in this section. In the first problem, a reactor and a reaction system is studied and based on the results from the simulation an optimum design on the reactor geometry is proposed. A combined system of fluid flow equations together with convection, diffusion and reaction equations for mass transfer has been considered. The simulations are carried out with the help of COMSOL.

Second example in this section is a fluid flow simulation in a capillary die. The capillary die is a device simulating the fluid flow in an injection moulding process. The pressure in the capillary changes with time until it reaches the steady state situation. Perturb continuity scheme has been chosen to solve this problem.

5.2.1 Optimum reactor design for the phenol production

A ‘reactor’ in which chemical transformation takes place, has to carry out several functions such as bringing reactants into intimate contact (to allow chemical reactions to occur), providing an appropriate environment (temperature and concentration fields, catalysts) for an adequate time and allowing for the removal of products. In order to reach the optimum reactor design, the following factors should be considered: cost, product quality, safety, environmental impact, conversion, selectivity, stability and operatability.

In the present work, two reactor systems namely the membrane and plug flow reactor, have been used to produce phenol (Figure 5-4). The main goal of the simulation is to study the effects of geometrical parameters such as reactor length and diameter together with operational parameters such as inlet flow rate and concentration on efficiency of the reactor. The results from the two reactors have been compared. Finally, the optimum design for the reactor has been suggested.
5.2.1.1 Modelling membrane tube

The membrane reactor was modelled to predict the influence of the geometrical parameters on the production of phenol. Figure 5-5 schematically shows the reactors geometry and specified boundary conditions. All the simulations were carried out at isothermal conditions. Table 5-1 shows the numerical values of the parameters used in the simulation.

<table>
<thead>
<tr>
<th>Reaction constant $(\text{mol}/\text{m}^3\text{h})$</th>
<th>Benzene inlet velocity $(\text{m/s})$</th>
<th>Inlet hydrogen velocity $(\text{mol}/\text{m}^3)$</th>
<th>Dynamic viscosity $(\text{Ns}/\text{m}^3)$</th>
<th>Inlet benzene concentration $(\text{mol}/\text{m}^3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.32e-3</td>
<td>0.01</td>
<td>0.001</td>
<td>0.008</td>
<td>10</td>
</tr>
</tbody>
</table>

The conversion of benzene to phenol in a 30mm long reactor with the cross section diameter of 3 mm was modelled. Also, the modelling was carried out when a solid
cylinder with 1 mm in diameter is inserted into the tube. The latter case results in an annulus shape geometry.

To validate the constructed model, the results generated by the simulation are compared with the results from the experiments. Table 5-2 shows the comparison of the simulated and experimental results for the conversion of benzene with and without the inner solid cylinder.

![Diagram of reactor geometry and boundary conditions](image)

Table 5-2 Experimental and simulation results [phenol (mmol/h)]

<table>
<thead>
<tr>
<th></th>
<th>Without the inner tube</th>
<th>With the inner tube of 1 mm diameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Simulations</td>
<td>1.8</td>
<td>2.3</td>
</tr>
</tbody>
</table>

Figure 5-5 Schematics of the reactor geometry and the specified boundary conditions.
(a) Membrane reactor
(b) Plug flow reactor

Table 5-2 Experimental and simulation results [phenol (mmol/h)]
Based on the agreement between simulated and experimental results, the proposed model was employed to study the effect of the reactor tube length on the conversion of benzene to phenol. Figure 5-6 shows the concentration of the produced phenol and conversion of benzene versus the tube length, respectively. As it can be seen in Figure 5-6, an increase in the tube length results in an increase of phenol production up to the tube length of 60 mm above which the increase in tube length decreases the production of phenol. This length is considered to be the optimum length at which the production of phenol is maximised.

For the annular geometry, the effect of increasing the inserted solid cylinder diameter on the conversion of phenol has been investigated. Figure 5-7 shows the conversion of benzene versus the annulus thickness (the area between the tube and inserted solid cylinder). Increasing the diameter of the inserted solid cylinder results in narrower annulus that increases the benzene conversion.

![Figure 5-6 Concentration of phenol (X) and conversion of benzene (O) versus the tube length (Tube diameter = 3mm)](image)
Results and discussions

The effects of changing the flow rate and the composition of the reaction components on the product have also been investigated. As it is shown in Table 5-3, decreasing the flow rate results in higher phenol (product) concentration. Experimental results suggest the value of 0.01 m/s as an optimum inlet velocity. As it can be seen in Table 5-3, the inlet velocities lower than 0.01 m/s do not change the product concentration dramatically.

Table 5-3 Experimental and simulation results (Tube length = 30 mm, diameter = 3 mm)

<table>
<thead>
<tr>
<th>Inlet velocity (m/s)</th>
<th>0.0001</th>
<th>0.001</th>
<th>0.01</th>
<th>0.1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol concentration (mol/m²)</td>
<td>0.112</td>
<td>0.1106</td>
<td>0.092</td>
<td>0.037</td>
<td>0.0045</td>
</tr>
</tbody>
</table>

The simulations results show that increasing the inlet concentration of the reactants result in higher concentration of the product (phenol). Although, this factor increases the product concentration but also increases the risk of reaching flammability point and explosion in the system as well. On the other hand, returning (recycling) the benzene which is not converted to phenol from the outlet to the feed to be used again is an expensive process. Therefore, increasing the benzene concentration in the feed will result in an economically inefficient system. As a conclusion, the flow rate and concentration are not proper factors to be optimized just by the mathematical simulation due to the experimental limitations and considerations.

Figure 5-7 Conversion of benzene versus the annulus thickness (Tube length=30 mm)

The effects of changing the flow rate and the composition of the reaction components on the product have also been investigated. As it is shown in Table 5-3, decreasing the flow rate results in higher phenol (product) concentration. Experimental results suggest the value of 0.01 m/s as an optimum inlet velocity. As it can be seen in Table 5-3, the inlet velocities lower than 0.01 m/s do not change the product concentration dramatically.

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5.2.1.2 Modelling plug flow reactor

The second approach to produce phenol is using the plug flow reactor. In this approach the reactants flow in together from the same side and the reaction starts when they meet the catalyst which is packed in the middle of the tube. Mathematical model has been constructed based on the data provided by the experiments. Table 5-4 shows the experimental data.

Table 5-4 Parameters used in the simulation

<table>
<thead>
<tr>
<th>Reaction constant, $k_1$ (mol/m$^3$h)</th>
<th>Inlet velocity (m/s)</th>
<th>Inlet hydrogen concentration (mol/m$^3$)</th>
<th>Reaction constant, $k_2$ (mol/m$^3$h)</th>
<th>Inlet benzene concentration (mol/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.3e-3</td>
<td>0.028</td>
<td>4.54</td>
<td>1.85e-4</td>
<td>45.4</td>
</tr>
</tbody>
</table>

The experiments show the value of 1.86 (mol/m$^3$) for the concentration of phenol while the simulation’s value is 2.12 (mol/m$^3$). The agreement between simulated and experimental results confirmed the reliability of the constructed model. Figure 5-8 shows the concentration of phenol across the length of the reactor tube.

Figure 5-8 Concentration of phenol along the tube length
(Catalyst packed area length = 4 mm, diameter=3mm)
5.2.2 Conclusion

The modelling shows longer tubes increase the conversion of benzene but there is an optimum length because of preventing side reactions. The tube length of 60 mm results in the maximum rate of product. Also the modelling results show higher productivity using a solid tube inside the membrane. Due to the experimental restrictions the operational parameters can not be solely relied upon. As the modelling results show, the plug flow reactor results in higher amount of product.
Chapter 5 Results and discussions

5.2.2 Pressure study in a capillary rheometer

5.2.2.1 Aim

Based on the experimental results from the department of IPTME in the Loughborough University, a mathematical model is constructed to study the variation of pressure versus time in a capillary rheometer.

5.2.2.2 Physical Background

All materials, whether gas, liquid or solid exhibit some change in volume when subjected to a compressive stress. The degree of compressibility is measured by a bulk modulus of elasticity, $E$, defined as either \[ E = \frac{dp}{d\rho / \rho} \] or \[ E = \frac{dp}{(-dV / V)'} \], where $dp$ is a change in pressure and $d\rho$ is the corresponding change in density or specific volume. Since \[ \frac{dp}{d\rho} = c^2 \], where $c$ is the adiabatic speed of sound, another expression for $E$ is $E = \rho c^2$. In liquids and solids, $E$ is typically a large number so that density and volume changes are generally very small unless exceptionally large pressure is applied.

5.2.2.3 Mathematical model

In the present study the continuity equation representing a slightly compressible fluid is used in order to consider the effect of compressibility on pressure variation with time:

\[ \frac{1}{\rho c_i^2} \frac{\partial p}{\partial t} + \nabla \cdot (V) = 0 \] \hspace{1cm} (6-7)

where $\rho$ is fluid density, $p$ is pressure and $c_i$ is the speed of sound in the fluid.

The final working equations of the flow model have been derived using a U-V-P approach since the primary desired variable of interest in the computations is pressure.
drop. Second order Taylor Galerkin method in conjunction with theta time stepping method has been used to deal with transient nature of the problem [88,89].

Table 5-5 lists geometrical dimensions of the domain and physical parameters of the fluid.

<table>
<thead>
<tr>
<th>Table 5-5 Geometrical dimensions and physical properties of the fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Barrel diameter</td>
</tr>
<tr>
<td>Die radius (r)</td>
</tr>
<tr>
<td>Die length (L)</td>
</tr>
<tr>
<td>Power law index</td>
</tr>
<tr>
<td>Consistency constant (stress at 1/s)</td>
</tr>
<tr>
<td>Bulk modulus</td>
</tr>
</tbody>
</table>

The following values have been chosen for velocity of sound, time steps and theta parameter that provide the best fit to experimental data:

\[ c_l = 900 \text{ m/s}, \quad \Delta t = 0.1 \text{ s}, \quad \theta = 0.85 \]

The following input velocities have been selected in the present work:

<table>
<thead>
<tr>
<th>Table 5-6 inlet velocities (cm/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.78</td>
</tr>
</tbody>
</table>

The domain geometry is shown in Figure 5-9.
5.2.2.4 Results

The following Figures (5-10, 5-11 and 5-12) show the velocity and pressure profile in steady state situation. Pressure variation with time has been plotted and compared with experimental data in Figure 5-13.
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Figure 5-10 Velocity profile (m/s)

Figure 5-11 Velocity profile (m/s)
Figure 5-12 Pressure distribution (Pa)

Figure 5-13 Theoretical and experimental results-pressure (MPa) versus time (1/s)
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5.3 Fluid solid interaction

To study the system of fluid-solid interaction, two benchmark problems have been solved and the sensitivity of the system to different properties of solid and fluid has been investigated. In the first example, Figure 5-14 shows a 2D solid wedge which is in interaction with a fluid. A complex geometry has been chosen here to study the ability of the program to deal with complex geometrical systems. Also a 3D model of a flow meter has been considered and solved in this section.

5.3.1 Case Study – 2D Wedge

A problem with the complex geometry (Figure 5-14) has been considered to study the fluid-solid interaction problem. Pressure at the outlet in the right and left side of fluid domain restricted to be zero. Velocity value applied at the fluid bottom is 0.3 cm/sec. solid displacement at top is fixed. The fluid has the following properties: viscosity =0.01 dyn.cm and density =1 gr/cm³. The solid was considered to be either elastic and rigid with the properties listed Table 5-7.
Figure 5-14 the problem geometrical dimensions

Table 5-7 elastic and rigid solid properties

<table>
<thead>
<tr>
<th>Solid- Elastic</th>
<th>Solid-rigid</th>
</tr>
</thead>
<tbody>
<tr>
<td>E=5000 Pa</td>
<td>E=2.7 e10 Pa</td>
</tr>
<tr>
<td>Poisson’s ratio =0.49</td>
<td>Poisson’s ratio =0.3</td>
</tr>
</tbody>
</table>

The solution results for the elastic solid are shown in the following figures: 5-15, 5-16 and 5-17.
Figure 5-15 displacement profile (m) and distribution of Von Misses stress (Pa) in the solid wedge
Figure 5-16 pressure (pa) and velocity profile (m/s) in the fluid domain
Figure 5-17 normal stress distribution in X and Y direction in the solid wedge (Pa)
The results for the rigid solid are shown in figures 5-18, 5-19 and 5-20:

Figure 5-118 displacement profile (m) and distribution of Von Misses stress (Pa) in the solid wedge
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Figure 5-129 pressure and velocity profile in the fluid domain (Pa)
Figure 5-20 normal stress distribution in X and Y direction in the solid wedge (Pa)
5.3.2 simulation of flow past an obstacle (3D) – Flow-meter

In this model, fluid is flowing through a channel with a flexible obstacle. Due to the viscous and pressure forces exerted by the fluid, the obstacle is bending. With the obstacle undergoing a large deformation, the fluid flow domain is also changing considerably. Simulations are taking these changes into account by computing the flow field on a moving mesh attached to the obstacle.

In this example, the dimensions are such that the setup mostly resembles a flow-meter, but the modeling principles used are very general and can be applied to many situations where there is interaction between a structure and a fluid flow domain.

Model Definition

In this example, the flow channel is 200 µm long, 150 µm high and 150 µm wide. A flag-shaped obstacle has a slightly off-center position in the channel. The fluid is water with a density of $\rho = 1000$ kg/m$^3$ and dynamic viscosity of $\mu = 0.001$ pa.s. The obstacle is made of a flexible material with a density of $\rho = 7850$ kg/m$^3$ and a Young's modulus of $E = 8$ MPa.
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The model consists of a fluid part, solved with the Navier-Stokes equations in the flow channel, and a structural mechanics part, which is solved in the obstacle. A Moving Mesh makes sure the flow domain is deformed along with the obstacle.

5.3.2.1 Fluid flow

The fluid flow in the channel is described by the Navier-Stokes equations. The Navier-Stokes equations are solved in the spatial (deformed) coordinate system. At the inlet, the model uses a fully developed laminar flow. Zero pressure is applied at the outlet. No-slip boundary conditions are used at all other boundaries. Note that this is a valid condition only as long as you are solving the stationary problem. In a transient version of the same model, with the obstacle starting out from an undeformed state, it is necessary to state that the fluid flow velocity is the same as the velocity of the deforming obstacle.

5.3.2.2 Structural mechanics

The structural deformations are solved by using an elastic and a nonlinear geometry formulation to allow large deformations.

For boundary conditions, the obstacle is fixed to the bottom of the fluid channel so that it cannot move in any direction. All other boundaries experience a load from the fluid which is the sum of pressure and viscous forces.

5.3.2.3 Moving Mesh

The motion of the deformed mesh is modeled using Winslow smoothing (Appendix2). The boundary conditions control the displacement of the moving mesh with respect to the initial geometry. At the boundaries of the obstacle, this displacement is the same as the structural deformation. At the exterior boundaries of the flow domain, it is set to zero in all directions.
Figure 5-22 (a) solid displacement in x direction (m) (b) fluid velocity field (m/s)

Total number of elements which has been used for this model are as follows: 1346 tetrahedral elements (1135 for the fluid domain and 211 for the solid part) and 396 87
triangle elements as boundary elements. Von mises and Tresca stresses shows the maximum values of 5.41e5 and 5.84e5 Pa, respectively.

Figure 5-23 pressure profile (Pa)
5.4 Fluid porous solid interaction

In the present section, fluid-porous solid interaction systems are studied. Stress-strain behaviour of solid has been studied to investigate how solid structure performs under working conditions.

5.4.1 Case study 1

First case study is an example of fluid-solid interaction system in which the solid can be either porous or non-porous. The solid structure domain is located on the side of fluid flow path (Figure 5-24). This case study resembles the cross flow filters if the solid considered is a porous one.

![Figure 5-24 case study 1 geometry](image)

A plug flow Dirichlet velocity boundary with an average velocity value of 0.01 (m/s) is specified on $\square_{AB}$. No-slip wall condition is imposed on the solid walls by making both velocity components on the wall to be zero. Stress free boundary condition is imposed on the exit boundary $\square_{CD}$. The fluid domain width and length are 0.01 m and 0.1 m, respectively. The solid-fluid interaction boundary conditions have been imposed on the interface $\square_{EF}$. The dynamic viscosity of the fluid is 80 Pa.s and the young's modulus and Poisson's ratio are $2\times10^5$ and 0.3, respectively. The problem first discretized into 142 triangular elements. The number of elements was then increased to gain more accurate results. The optimum number of elements was chosen to be 2272 which compromises the simulation time and accuracy of simulation.
5.4.1.1 Results and discussion

The viscous and total force applied to the solid part in the y direction were calculated to have the following values, 0.005244 N and 30.400306 N. The stated force results in the total displacement of 5.5*10^{-4} m in the solid object. Fluid inlet velocity is one of the factors that affect the displacement of the solid domain. The results from this investigation are shown in Table 5-8. The effect of the viscosity variation on the displacement of the solid object was also studied. Keeping all the parameters and reducing the viscosity by one and two order of magnitude results in displacement of 5.9038*10^5 m and 5.926*10^6 m in the solid object. The calculated viscous and total forces in y direction reads the following values, 2.537*10^7 N and -0.312029 N, respectively. The solid object’s Poisson’s ratio was then changed to study its effect on the displacement of the solid object (Table 5-9). Increasing the young’s modulus of the solid results in less displacement in the solid object.

To investigate how the geometrical factors would affect the displacement of the solid, the exit (CD) was half blocked. This resulted in increasing of the outlet flow velocity and the solid displacement value of 9.393e^{-4} m.

Table 5-8 Displacement (m) of solid interface with fluid versus fluid inlet velocity

<table>
<thead>
<tr>
<th>Velocity(m/s)</th>
<th>0.001</th>
<th>0.005</th>
<th>0.01</th>
<th>0.015</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement(m)</td>
<td>5.903e-5</td>
<td>2.89e-4</td>
<td>5.50e-4</td>
<td>8.05e-4</td>
<td>2.07e-3</td>
</tr>
</tbody>
</table>

Table 5-9 Displacement (m) of solid interface with fluid versus Poisson ratio

<table>
<thead>
<tr>
<th>Poisson ratio</th>
<th>0.1</th>
<th>0.2</th>
<th>0.4</th>
<th>0.499</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement(m)</td>
<td>5.61e-4</td>
<td>5.63e-4</td>
<td>5.50e-4</td>
<td>5.24e-4</td>
</tr>
</tbody>
</table>

Figure 5-25 shows the displacement in the solid. The distributions of Von-mises and Tresca stresses in the solid domain are shown in Figure 5-26 where the most probable area in the solid for failures is the points where the stresses have the maximum values. The maximum calculated values for the Von-Mises and Tresca stresses are 2.97e4 Pa and 3.24e4 Pa, respectively.
Figure 5-25 displacement in the solid (m)

(a)
For the present case study, if the solid domain considered is a porous medium then it resembles the cross flow filtration process. Here, Permeability of the porous domain plays the role of a controller for the direction of the flow. Figure 5-27 shows the velocity profile with different values of permeability. Also displacement of the interface has been calculated and results are presented in Table 5-10.

Table 5-10 Displacement (m) versus permeability (m²) of porous domain

<table>
<thead>
<tr>
<th>Permeability(m²)</th>
<th>1e-5</th>
<th>1e-6</th>
<th>1e-7</th>
<th>1e-8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement(m)</td>
<td>7.48e-5</td>
<td>2.869e-4</td>
<td>5.15e-4</td>
<td>5.71e-4</td>
</tr>
</tbody>
</table>
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(a)

(b)
Figure 5-27 velocity profile with different values of permeability (m²)
(a) 1e-5 (b) 1e-6 (c) 1e-7 (d) 1e-8
5.4.2 Case study 2

The second case study is an example of solid-fluid interaction in which the porous solid medium is located along side the fluid domain. Figure 5-28 shows a schematic representation of the geometry of the case study 2. This is a simple model of a dead-end filter.

![Figure 5-28 case study 2 geometry](image)

A plug flow Dirichlet velocity boundary condition with an average velocity value of 0.01 (m/s) is specified on \( \square_{AB} \). No-slip wall boundary condition is imposed on the solid walls by making both the velocity components on the wall to be zero. Stress free boundary conditions are imposed on the exit boundary \( \square_{EF} \). The fluid domain width and length are 0.01 m and 0.1 m, respectively. The solid-fluid interaction boundary conditions have been imposed on the interface \( \square_{CD} \). The dynamic viscosity of the fluid is 80 Pa.s and the young’s modulus and Poisson’s ratio are \( 2e^6 \) and 0.3, respectively. The permeability of the porous domain is \( 1e^{-7} \) m\(^2\).

5.4.2.1 Results and discussions

The pressure drop along the domain is \( 1.855e^5 \) Pa while the maximum displacement of the porous solid interface domain is \( 5.163e^{-4} \) m. Figure 5-29 shows the pressure distribution in the domain. The simulation results show that changing viscosity values would significantly affect the porous solid displacement and the pressure drop. The calculated pressure drop and maximum displacement due to different viscosities are listed in Table 5-11. One factor which has a significant effect on the deformation of the porous domain is the porous domain permeability. Table 5-12 shows maximum displacement of porous interface with different values of permeability. As it is shown in the Table 5-12, lower permeability results in higher deformation in the solid domain due to the higher pressure drop. Figure 5-30 shows the pressure drop distribution in the domain when the permeability is \( 1e^{-6} \) m\(^2\).
Figure 5-29 pressure distribution (Pa)

Table 5-11 Variations of pressure drops and maximum porous interface displacements for fluids with different viscosities

<table>
<thead>
<tr>
<th>Viscosity (Pa.s)</th>
<th>80</th>
<th>8</th>
<th>0.8</th>
<th>0.08</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure drop (pa)</td>
<td>1.85e5</td>
<td>1.88e4</td>
<td>1886.9</td>
<td>188.7</td>
</tr>
<tr>
<td>Displacement (m)</td>
<td>5.163e-4</td>
<td>4.75e-5</td>
<td>4.71e-6</td>
<td>4.71e-7</td>
</tr>
</tbody>
</table>

Table 5-12 Variations of maximum porous interface displacements for porous solid with different permeability

<table>
<thead>
<tr>
<th>Permeability (m²)</th>
<th>1e-5</th>
<th>1e-6</th>
<th>1e-7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement (m)</td>
<td>1.035e-5</td>
<td>5.56e-5</td>
<td>5.16e-4</td>
</tr>
</tbody>
</table>
When the fluid domain is divided into a porous and non-porous domain, special consideration should be made about meshing the porous domain. The domain was meshed with 132, 528 and 2112 triangular elements. The results in Figure 5-31 suggests, only the finest mesh (with 2112 triangle elements) would yield stable results.
There is an alternative to the use of a finer mesh and that is based on using the polynomial with higher degree as an interpolation function or using special group of
element named Bubble elements. A detailed information on Bubble elements can be found in the literature [90].

The following figure shows the maximum Von Mises stress versus the permeability in the porous medium.

![Figure 5-32 maximum Von-mises stress (Pa) versus permeability (m²)](image)

*Figure 5-32 maximum Von-mises stress (Pa) versus permeability (m²)*
To look at this problem from another point of view, a gap was then located in the solid walls, where part of the fluid may leave the domain before reaching the porous medium. This is shown schematically in Figure 5-33.

![Figure 5-33 case study 2 geometry](image)

The flow and solid properties are as follows:

- Density = 1000 kg/m\(^3\)
- Viscosity = 80 pa.s
- Inlet velocity = 0.01 m/s
- Modulus of elasticity = \(2 \times 10^6\) Pa
- Poisson's ratio = 0.33
- Permeability = \(1 \times 10^{-8}\) m\(^2\)

Calculations based on the above properties show the maximum porous interface displacement and fluid pressure drop values to be \(2.38 \times 10^{-5}\) m and \(2.105 \times 10^4\) pa, respectively. Table 5-13 shows how changing the permeability affects the maximum displacement and pressure drop for this problem. Conclusions based on the data from Table 5-13 is that for this case, the change in permeability does not have a significant effect on the displacement of the porous interface. At lower permeabilities the fluid tends to leave the domain from the gap (Figure 5-34).

**Table 5-13 displacement versus permeability of porous domain**

<table>
<thead>
<tr>
<th>Permeability (m(^2))</th>
<th>1e-7</th>
<th>1e-8</th>
<th>1e-9</th>
<th>1e-12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement (m)</td>
<td>2.09e-5</td>
<td>2.38e-5</td>
<td>2.49e-5</td>
<td>2.52e-5</td>
</tr>
</tbody>
</table>
The results show one order of magnitude reduction in the displacement as the modulus of elasticity increases by one order of magnitude. Figure 5-35 shows the displacement results with different values of Poisson's ratio. A solid material with a Poisson's ratio of 0.499 is considered to be nearly incompressible because the value of 0.5 results in fully incompressible solid.
Considering the solid to be non-porous and the gap as the only boundary area where the fluid may leave the domain, the problem is studied with the fluid having different rheological behaviour. Power-law model has been chosen to account for the non-Newtonian behaviour of the fluid. With the power-law index set to 1, and values less than and greater than 1, when the flow is expected to show Newtonian, shear thinning and shear thickening behaviour, respectively. With the inlet velocity of 0.01 m/s, Poisson’s ratio equal 0.33 and modulus of elasticity of $2\times 10^6$ Pa the following results have been predicted for the maximum displacement of the solid which happens at the
interface. Based on the following values of Power-law index 0.7, 1 and 1.1, the following maximum interface displacement of 9.493e\(^{-6}\) m, 2.483e\(^{-5}\) m and 3.45e\(^{-5}\) m have been predicted respectively. The pressure drops across the domain shows the following values depending on different rheological behaviour of the fluid.

\[ n = 0.7 \quad \text{Pressure drop} = 1.017 \times 10^4 \]
\[ n = 1 \quad \text{Pressure drop} = 2.15 \times 10^4 \]
\[ n = 1.1 \quad \text{Pressure drop} = 2.803 \times 10^4 \]

The forces from the fluid on the solid interface for different values of Power-law index are as follows:

\[ n = 1 \quad \text{Viscous force} = 0.00080537 \text{ N} \]
\[ \text{Total force} = 0.8626 \text{ N} \]

\[ n = 0.7 \quad \text{Viscous force} = 0.00001903 \text{ N} \]
\[ \text{Total force} = 0.3239 \text{ N} \]

\[ n = 1.1 \quad \text{Viscous force} = 0.001773 \text{ N} \]
\[ \text{Total force} = 1.204217 \times 10^3 \text{ N} \]
5.4.3 Case study 3

In fixed bed reactors, the catalyst is usually packed in the middle of the reactors where reaction starts as soon as reactants pass through it. The geometry consists of two free flow domains and a porous domain in the middle, as it is shown in Figure 5-36.

Fluid entering the domain from the left side (\(\overline{AB}\)) and pass through the porous domain and exit the domain from the right (\(\overline{GH}\)). No slip boundary condition applied to the side wall and the pressure at the exit set to be zero. The fluid with the viscosity of 80 Pa.s and the density of 1000 kg/m\(^3\) enters as a plug flow with the velocity of 0.005 m/s. The porous domain is specified with the permeability of \(1e^{-8}\) m\(^2\) and young's modulus and Poisson's ratio of \(2e^6\) Pa and 0.33, respectively. Figure 5-37 shows the pressure and velocity distribution.
For this case study, different values of permeability have been tried and the resultant pressure drops have been calculated. The results are shown in Table 5-14.

Table 5-14 variations of Pressure drop and maximum displacement of the interface with different values of permeability

<table>
<thead>
<tr>
<th>Permeability (m²)</th>
<th>1e-5</th>
<th>1e-6</th>
<th>1e-7</th>
<th>1e-8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement (m)</td>
<td>4.171e-6</td>
<td>1.44e-5</td>
<td>1.106e-4</td>
<td>1.093e-3</td>
</tr>
<tr>
<td>Pressure drop (pa)</td>
<td>5170</td>
<td>7102</td>
<td>2.496e4</td>
<td>1.874e5</td>
</tr>
</tbody>
</table>

Figure 5-38 shows the pressure distribution with the permeability values of 1e-6 and 1e-7.
(a) permeability = 1e-6 m$^2$
Figure 5-14 pressure distribution in the domain with different value of permeability for porous media (pa)

(b) permeability $1e-7 \text{ m}^2$
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Calculation of Von-Mises and Tresca stresses show the following values:

Vonmises stress $2.54 \times 10^6$ Pa, Tresca stress $2.57 \times 10^6$ Pa

The second Piola-Kirchoff stress in x and y direction has been calculated. Figure 5-39 show the distribution and values of the stated stresses in the solid domain.

(a)
Figure 5-39 Second piola-kirchhoff stress in x and y direction (pa)
5.4.4 Case study 4

In many fluid-solid interaction problems, a slender solid is positioned in the fluid path while being displaced and deformed due to the force exerted by the fluid. Solution to this problem is similar to that of problems in real life such as Heart valve.

A plug flow Dirichlet velocity boundary with an average velocity value of 0.001 (m/s) is specified on $\Box_{AB}$. No-slip wall boundary condition is imposed on the solid walls by making both the velocity components on the wall to be zero. Stress free boundary condition is imposed on the exit boundary $\Box_{CD}$. The fluid domain width and length are
0.2e-4 m and 1e-4 m, respectively. The solid-fluid interaction boundary conditions have been imposed on the interface boundaries. The dynamic viscosity of the fluid is 0.1 Pa.s and the young's modulus and Poisson's ratio are 2e^5 Pa and 0.3, respectively.

5.4.4.1 Results and discussions

The solid displacement is shown in Figure 5-41. The maximum displacement that happens on the edge of solid bar is 9.489e-6 m. The velocity and pressure profiles are shown in Figures 5-41 and 5-42.

![Figure 5-41 solid displacement (m)](image-url)
Figure 5-42 (a) velocity, m\text{s}^{-1} and (b) pressure, Pa distributions
To study the variations of fluid flow and solid domain properties on the system response, the following boundary conditions and fluid properties have been defined for the present problem. A plug flow velocity in Y direction with the value of 0.0001 m/s has been defined. The no-slip boundary condition has been applied on the flow domain. Young's modulus and Poisson's ratio for the solid structure are 2e6 Pa and 0.33, respectively. The fluid is considered to be non-Newtonian following power-law model. The consistency coefficient and power-law index are 0.1, 1.1, respectively. This system simulation shows 2.007e-6 m for the maximum displacement of solid which occurs on the edge of the solid bars. As it is shown in Figure 5-43, the maximum Von-mises stress value is 1.264e5 pa. The value of 1 for the power-law index, results in Newtonian behaviour of the fluid. For this case the maximum displacement shows the value of 1.295e-6 m while the maximum Von-mises stress is 7.94e4 pa. To study the system response when the fluid shows the shear thinning behaviour, the power-law index was set to have a value of 0.9. The predicted maximum displacement and maximum Von-mises stress had the following values of 7.3e-7m, and 4.28e4 Pa, respectively. The calculations showed that higher modulus of elasticity results in less displacement in the solid bars.
Figure 5-43 Von-mises stress in the solid domain (Pa)
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Geometrical factors play a key role in designing the systems. For the present case, the effect of changing the solid object (solid bar) width and length has also been investigated. Solid length reduced to 0.6 e-6 m and its width increased to 2.5 e-6 m. Therefore the resultant solid bars had the following dimensions: 0.9e-6 * 1.5e-6 and
0.6e-6 * 2.5e-6 m. The results reveal that the shorter bar results in decreasing the value of maximum von mises stress and displacement. On the other hand, increasing the solid bar width results in increasing the maximum displacement and von misses stresses.

For the fluid with shear thickening behaviour, if the young’s modulus of the solid and consistency coefficient decrease by one order of magnitude and set to the values of \(2e5\) Pa and \(0.01\) Pa.s, respectively then the maximum displacement in solid bars will be \(2 \times 10^{-6}\) m. the predicted maximum Von-mises and Tresca stresses show the following values:

\[
\text{Von misses stresses} = 1.26e4 \text{ Pa} \\
\text{Tresca stresses} = 1.4 \times 10^4 \text{Pa}
\]
5.5 New approaches to the fluid-solid interaction problems

5.5.1 Steady state Fluid flow-elastic solid interaction system

Based on the discussions given in chapter 4, and the derivation of a unique set of equations for the interaction of a viscous fluid and elastic solid, Stokes equation and the equation of elastic solid with small strain and displacement are considered for the fluid and solid domains, respectively. Continuous Penalty scheme has been used to satisfy the LBB condition in the solution of incompressible fluid flow equations. The problem domain geometry and boundary conditions are shown in Figure 5-45. The inlet velocity is 0.1 m/s (in +y direction), no-slip boundary condition has been defined for the solid walls in the fluid region. Zero displacement on the side walls in the solid region has been considered.

Shear viscosity in fluid equations is defined by the power-law model as

$$\eta = \eta_0 (\dot{\gamma})^{n-1}$$

where $\eta_0$ is the consistency coefficient, $\dot{\gamma}$ is the shear rate and $n$ is power-law index.

Although equations for the fluid and solid are the same in this case, but on the interface boundary a nodal displacement method (as discussed in chapter 4) need to be performed due to unequal boundary integrals.
Chapter 5 Results and discussions

Figure 5-45 problem geometry and boundary conditions

Table 5-15 Numerical values of physical parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho ) (solid)</td>
<td>9800 kg m(^{-3})</td>
</tr>
<tr>
<td>( \rho ) (fluid)</td>
<td>1000 kg m(^{-3})</td>
</tr>
<tr>
<td>( \eta_0 )</td>
<td>88700 kg m(^{-1}) s(^{-1})</td>
</tr>
<tr>
<td>( E )</td>
<td>2, 20, 200 Mpa</td>
</tr>
<tr>
<td>( \nu )</td>
<td>0.19, 0.29, 0.4, 0.499</td>
</tr>
</tbody>
</table>
5.5.1.1 Results and discussion

Variations in physical and mechanical parameters in fluid and solid equations lead to different results in deformation of solid medium. The effects of increasing the elasticity modulus on deformation of interface between solid and fluid is shown in Figure 5-46. Figure 5-47 shows the deformation of solid material at the interface as rheological behaviour of fluid changes due to variations in power-law index. As the power-law index of the fluid flow decreases, its velocity increases. This results in a higher deformation in the solid phase. Therefore, the highest solid deformation occurs when the power-law index of the interacting fluid is less than unity. Figure 5-48 shows the displacement of interface with the variation of Poisson’s ratio. As is shown in these figures, the rheological behaviour of the fluid has a significant effect on the deformation of the solid interface. Similarly, as the Poisson ratio approaches 0.5, the solid interface becomes less deformed. This is because for Poisson ratio of 0.5, the solid should behave as an incompressible medium. As expected for a higher modulus of elasticity, a reduction in the deformation of the interface between the solid and fluid phases has been observed.
Figure 5-46 Interface displacement with different values for solid elastic modulus (m)

Figure 5-47 Interface displacement with different rheological behavior of the fluid (m)
Figure 5.48 interface displacement with different values for Poisson's ratio of the solid (m)
5.5.2 Steady state Fluid flow-porous solid interaction system

Fluid-porous solid interaction phenomena can be detected in many applications and natural systems. Unfortunately, there has not been a vast literature on this subject and this interaction hasn’t been incorporated in any commercial modelling software.

The distinct point in modelling the interaction of the fluid and porous solid is that the fluid flow equation has to be solved in the porous media as well. Therefore, the free fluid flow and porous flow equations have to be connected on the interface. To model the fluid flow in the porous medium, Darcy equation is selected due to low value of the permeability.

5.5.2.1 Case study

As it is shown in Figure 5-49, a rectangular domain has been selected for the problem geometry. Fluid with the inlet velocity of 0.1 m/s enters domain from the ‘AB’ side and then reach the porous domain at the interface ‘CD’ and deform the porous domain when passing through it. The physical and mechanical properties of the system are shown in Table 5-16.

The U-V-P scheme with Taylor-Hood element has been used for the fluid flow to satisfy the LBB condition. The domain discretized into 2000 elements. The 9-noded Lagrangian element has been selected for the modelling.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>1000 kg m(^{-3})</td>
</tr>
<tr>
<td>( \eta )</td>
<td>80 Pa.s</td>
</tr>
<tr>
<td>( E )</td>
<td>10 Mpa</td>
</tr>
<tr>
<td>( \nu )</td>
<td>0.3</td>
</tr>
<tr>
<td>( k )</td>
<td>1e-10</td>
</tr>
</tbody>
</table>
5.5.2.2 Solution strategy

(a) Partitioned

As discussed in previous chapters the fluid flow part is solved in the first step when the Stokes equation is connected to Darcy equation at the interface. The fluid stress that is exerted on the interface is then calculated. In the next step, the calculated stress is applied on the porous solid domain to calculate the displacement. The effects of changing the geometry on the fluid flow, due to the solid deformation, can be neglected, so the present problem is considered as a one way coupling. Figure 5-50 shows the velocity profile in the problem geometry. In addition, the pressure profile is shown in Figure 5-51.
Figure 5.50 velocity profile in the fluid-porous solid system (m/s)
(b) Direct coupling:

This is the same as the previous case study but the fluid flow (Stokes) equation is connected to equations of porous solid deformation at the interface through the
method discussed in chapter 4. Figures 5-52 and 5-53 show the interface displacement based on using portioned and direct coupling methods, respectively.

Figure 5-52 Interface displacement in y direction (m), partitioned method
Figure 5-53 Interface displacement in y direction (m), direct coupling method
Figure 5-54 schematic of the geometry after the porous medium deformation
Conclusions
Both partitioned and direct coupling procedures have been used to study the present problem. For this problem, the two stated methods show similar results. However, a longer time is spent on modelling using the partitioned method. To model complicated problems the partitioned method is more useful and can be utilized in conjunction with a powerful commercial software such as FLUENT (ANSYS).
Conclusions and scope for future work

6.1 conclusions

6.1.1 Fluid flow Modelling

A mathematical model is constructed based on the weighted residual finite element method to model the fluid flow systems. Three schemes, namely the continuous Penalty method, artificial compressibility scheme based on the use of nine-noded $C^0$ continuous Lagrange elements and a mixed formulation based on Taylor-Hood elements have been utilized. All the above methods yield reliable and stable results in the modelling of incompressible fluid flow in both porous and non-porous media. In particular, for the combined Stokes/Darcy flows, the third scheme gives stable and reliable results without such problems as numerical locking. Furthermore, this scheme is specifically well suited for the linking of the Stokes and Darcy regimes which can be done without imposition of any artificial boundary conditions at the free/porous interface. Computational meshes used in all three schemes should be more refined near the interface as compared to the other zones in a coupled domain.

6.1.2 Fluid-solid interactions

Two strategies namely, direct coupling and sequential coupling have been used in the present study to couple the fluid flow to porous or non-porous solid deformation equations.

For direct coupling, system of fluid-non-porous solid interaction is modelled using an in house developed scheme. This is applied to solve Stokes flow and linear elastic equations, conjunctively, thus modelling both fluid flow and solid deformation. In this method, combination of fluid flow and solid deformation equations as a coupled system provides a means for representing a unique set of equation for the entire domain. This approach is flexible and can be switched from fluid analysis to solid deformation modelling. This results in a significant reduction in computational cost.
However, this procedure exclusively depends on the use of continuous Penalty method with restriction on the value of the penalty parameter which should be related to the Young’s modulus and Poisson’s ratio of the solid phase.

All of the developed schemes satisfy the condition for the coupling of the solid deformation and fluid flow equations. Therefore using the developed scheme, Stokes and linear elastic equations are solved conjunctively under realistic boundary conditions and physical parameters. Variations in the physical and mechanical parameters in fluid and solid equations lead to different results in deformation of solid medium. As the power-law index of the fluid flow decreases, its velocity increases. This results in a higher deformation in the solid phase. Therefore, the highest solid deformation occurs when the power-law index of the interacting fluid is less than unity. From these results, it can be concluded that the rheological behaviour of the fluid has a significant effect on the deformation of the solid interface. Similarly, as the Poisson’s ratio approaches 0.5, the solid interface becomes less deformed. This is because for Poisson’s ratio of 0.5, the solid should behave as an incompressible medium. As expected for a higher modulus of elasticity, a reduction in the deformation of the interface between the solid and fluid phases has been observed.

Partitioned method has also been used in the present research study to model fluid-porous solid and fluid-non porous solid interaction. Solution to the system of fluid-nonporous solid interaction has been attempted through using commercial software, COMSOL. The Von-mises and Tresca stresses have been calculated in the deformed solid and based on their values the safety of the solid structure working under such applied conditions has been assessed.

Finally, the fluid-porous solid interaction system has been modelled with the stated software using the Brinkman equation for the fluid flow domain. This is because COMSOL cannot connect the free flow and Darcy equations in a straightforward manner. The main problem is the fundamental incompatibility of the two sets of
equations where one set (i.e. Stokes) contains a second order differential while Darcy’s equation is a first order partial differential equation. Therefore, the in-house developed software that resolves this problem is mathematically superior.

6.2 Suggestions for the Future works

The results presented in this study provide a basis to proceed with future investigations. Therefore, this work can be extended to examine a number of effects not covered in this study.

1- The model can be extended to solve 3D problems.

2- The model can be applied in more complex geometries such as those found in pleated cartridge filters. This is specifically important in the case of direct coupling.

3- Effects of temperature and heat transfer can be considered in the modelling as usually such systems operate under non-isothermal conditions.

4- Variations of permeability should be considered in the simulations. Change in the permeability occurs as a result of changing porosity due to the compression of porous medium. This effect is always present in a fluid flow - porous solid deformation.

5- The COMSOL package cannot solve a fluid/porous solid system in which part of fluid passes through the solid structure without considering unrealistic assumption about the structure and permeability of the porous domain. Fluid flow is assumed to follow Brinkman equations and effective viscosity is assumed to be the same as real fluid viscosity.
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Appendix 1

1- Arbitrary-Lagrangian Eulerian methods

2- Stress analysis in solid
**Arbitrary Lagrangian-Eulerian methods**

The numerical simulation of multidimensional problems in fluid dynamics and nonlinear solid mechanics often requires coping with strong distortions of the continuum under consideration while allowing for a clear delineation of free surfaces or fluid-structure interfaces.

The algorithm of continuum mechanics usually make use of two classical descriptions of motion: the Lagrangian description and Eulerian description. Because of the shortcomings of purely Lagrangian and purely Eulerian descriptions, a technique has been developed that succeeds, to a certain extent, in combining the best features of the both the Lagrangian and Eulerian approaches. Such a technique is know as arbitrary Lagrangian-Eulerian (ALE) description. In the ALE description, the nodes of the computational mesh may be moved with the continuum in normal Lagrangian fashion, or be held fixed in Eulerian manner, or, as suggested in Figure 1, be moved in some arbitrary specified way to give a continuous rezoning capability. Because of this freedom in moving the computational mesh offered by the ALE description, greater distortion of the continuum can be handled than would be allowed by purely Lagrangian method, with more resolution than that afforded by a purely Eulerian approach.
The majority of modern ALE computer codes are based on either finite volume or finite element spatial discretizations, the former being popular in the fluid mechanics area, the latter being generally preferred in solid and structural mechanics. The computer implementation of the ALE techniques requires the formulation of a mesh-updated procedure that assigns mesh-node velocities or displacements at each time step of a calculation. The mesh update strategy can be chosen by the user. However, the re-mesh algorithm strongly influences the success of the ALE technique and may represent a big burden on the user if it is not rendered automatic.
Two basic mesh-update strategies may be identified as mesh regularization and mesh-adaptation. The geometrical concept of mesh regularization can be exploited to keep the computational mesh as regular as possible and to avoid mesh entanglement during the calculation while a suitable indication of the error is required as a basic input to the re-mesh algorithm in mesh-adaptation technique.

In mesh regularization techniques, when the motion of the material surface (usually the boundaries) is known a priori the mesh motion is also prescribed a priori. This is done by defining an adequate mesh velocity in the domain, usually by simple interpolation. In general, this implies a Lagrangian description at the moving boundaries (the mesh motion coincided with the prescribed boundary motion), while a Eulerian formulation is employed far away from the moving boundaries. A transition zone is defined in between. The interaction problem between a rigid body and a viscous fluid studied by Huerta and Liu falls in this category. A method was proposed by Winslow in which the rezoning of the mesh nodes consists in solving a Laplace (or Poisson) equation for each component of the node velocity or position, so that on a logically regular region the mesh forms lines of equal potential. This technique has an important drawback: in a non-convex domain, nodes may run outside it. Techniques to precludes this pitfall either increase the computational cost enormously or introduce new terms in the formulation, which are particular to each geometry.
Stress analysis in solid

Stress analysis is an engineering discipline that determines the stress in materials and structures subjected to static or dynamic forces or loads (alternately, in linear elastic systems, strain can be used in place of stress).

The aim of the analysis is usually to determine whether the element or collection of elements, usually referred to as a structure, can safely withstand the specified forces. This is achieved when the determined stress from the applied force(s) is less than the ultimate tensile strength, ultimate compressive strength or fatigue strength the material is known to be able to withstand, though ordinarily a safety factor is applied in design.

A key part of analysis involves determining the type of loads acting on a structure, including tension, compression, shear, torsion, bending, or combinations of such loads.

Sometimes the term stress analysis is applied to mathematical or computational methods applied to structures that do not yet exist, such as a proposed aerodynamic structure, or to large structures such as a building, a machine, a reactor vessel or a piping system.

A stress analysis can also be made by actually applying the force(s) to an existing element or structure and then determining the resulting stress using sensors, but in this case the process would more properly be known as testing (destructive or non-destructive). In this case special equipment, such as a wind tunnel, or various hydraulic mechanisms, or simply weights are used to apply the static or dynamic loading.

When forces are applied, or expected to be applied, repeatedly, nearly all materials will rupture or fail at a lower stress than they would otherwise. The analysis to determine stresses under these cyclic loading conditions is termed fatigue analysis and is most often applied to aerodynamic structural systems.
**Maximum shear stress criterion**

Maximum shear stress criterion, also known as Tresca's or Guest's criterion is often used to predict the yielding of ductile materials.

Yield in ductile materials is usually caused by the slippage of crystal planes along the maximum shear stress surface. Therefore, a given point in the body is considered safe as long as the maximum shear stress at the point is under the yield shear stress $\sigma_y$ obtained from uni-axial tensile test.

With respect to 2D stress, the maximum shear stress is related to the difference in the two principal stresses. Therefore, the criterion requires the principal stress difference, along with the principal stresses themselves, to be less than the yield shear stress,

$$|\sigma_1| \leq \sigma_y, |\sigma_2| \leq \sigma_y, \text{ and } |\sigma_1 - \sigma_2| \leq \sigma_y$$

(1)

Graphically, the maximum shear stress criterion requires that the two principal stresses be within the green zone indicated below,

![Figure 1: Maximum shear stress criterion](image)

**Von mises criterion**

The von mises criterion also known as the maximum distortion energy criterion, octahedral shear stress theory, or Maxwell-Hencky-Von mises theory, is often used to estimate the yield of ductile materials.
The Von mises criterion states that failure occurs when the energy of distortion reaches the same energy for yield/failure in uni-axial tension. Mathematically, this is expressed as,

\[
\frac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2] \leq \sigma_y^2
\]  

(2)

In the case of plane stress, \(\sigma_3=0\). The von mises criterion reduces to,

\[
\sigma_1^2 - \sigma_1 \sigma_2 + \sigma_2^2 \leq \sigma_y^2
\]  

(3)

This equation represents a principal stress ellipse as illustrated in the following figure,

Also shown on Figure 2 is the maximum shear stress criterion (dashed line). This theory is more conservative than the Von mises criterion since it lies inside the Von mises ellipse.

In addition to bounding the principal stresses to prevent ductile failure, the Von mises criterion also gives a reasonable estimation of fatigue failure, especially in cases of repeated tensile and tensile-shear loading.
Maximum normal stress criterion

The maximum stress criterion, also known as the normal stress, coulomb, or Rankine criterion, is often used to predict the failure of brittle materials.

The maximum stress criterion states that the failure occurs when the maximum (normal) principal stress reaches either the uni-axial tension strength $\sigma_t$, or the uni-axial compression strength $\sigma_c$,

$$-\sigma_c / (\sigma_1, \sigma_2) / \sigma_t$$

(4)

Where $\sigma_t$ and $\sigma_c$ are the principal stresses for 2D stress.

Graphically, the maximum stress criterion requires that the two principal stresses lie within the green zone depicted below,

---

Mohr’s theory

The Mohr theory of failure, also known as the Coulomb-Mohr criterion or internal friction theory, is based on the famous Mohr Circle. Mohr theory is often used in predicting the failure of brittle materials, and applied to cases of 2D stress.
Mohr theory suggests that failure occurs when Mohr's Circle at a point in the body exceeds the envelope created by the two Mohr's circles for uni-axial tensile strength and uni-axial compression strength. This envelope is shown in the figure below,

![Mohr theory](image)

Figure 4 Mohr theory

The left circle is for uni-axial compression at the limiting compression stress of the material. Likewise, the right circle is for uni-axial tension at the limiting tension stress.

The middle Mohr circle on the figure (dash-dot-dash line) represents the maximum allowable stress for an intermediate stress state.

All intermediate stress states fall into one of four categories in the following table. Each case defines the maximum allowable values for the two principal stresses to avoid failure.

<table>
<thead>
<tr>
<th>Case</th>
<th>Principal Stresses</th>
<th>Criterion Requirements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Both in tension</td>
<td>$\sigma_1 &gt; 0, \sigma_2 &gt; 0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\sigma_1 &lt; \sigma_t, \sigma_2 &lt; \sigma_t$</td>
</tr>
<tr>
<td>2</td>
<td>Both in compression</td>
<td>$\sigma_1 &lt; 0, \sigma_2 &lt; 0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\sigma_1 &gt; -\sigma_c, \sigma_2 &gt; -\sigma_c$</td>
</tr>
<tr>
<td>3</td>
<td>In tension, in compression</td>
<td>$\sigma_1 &gt; 0, \sigma_2 &lt; 0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\frac{\sigma_1 + \sigma_2}{\sigma_t - \sigma_c} &lt; 1$</td>
</tr>
<tr>
<td>4</td>
<td>In compression, in tension</td>
<td>$\sigma_1 &lt; 0, \sigma_2 &gt; 0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\frac{\sigma_1 + \sigma_2}{-\sigma_c} &lt; 1$</td>
</tr>
</tbody>
</table>

Graphically, Mohr’s theory requires that the two principal stresses lie within the green zone depicted below,
Also shown on the Figure 5 is the maximum stress criterion (dashed line). The theory is less conservative than Mohr's theory since it lies outside Mohr's boundary.
A NUMERICAL METHOD FOR SOLID-LIQUID INTERACTION

Goodarz Khodabakhshi 1, Vahid Nassehi 2, Leila Shojaei 3, Richard J.Wakeman 4

Chemical Engineering Department
Loughborough University, Loughborough
Leicestershire, LE11 3TU,
United Kingdom

1 g.khodabakhshi@lboro.ac.uk
2 v.nassehi@lboro.ac.uk
3 l.shojaei@lboro.ac.uk
4 r.j.wakeman@lboro.ac.uk

Keywords: Solid-Fluid interaction, Finite element, Linear elastic solid, Stokes flow

Abstract. This paper deals with the mathematical modelling of coupled fluid flow and solid deformation problems. A novel mathematical technique for linking of the two sets of governing equations in a single model has been proposed. Results obtained by this technique using a range of power-law index for fluid flow simulation and elasticity modulus for the solid displacement are presented and discussed. Changing the rheological behaviour of the fluid has a significant effect on the deformation of the solid. These results are found to be self-consistent and as expected from a theoretical point of view.
1. INTRODUCTION

Simulation of solid-fluid interaction provides a challenging problem for computer modellers. Fluid flow and solid deformation modelling has been the subject of numerous research during the past few decades. Robust computer methods that provide reliable simulations for both these phases are now available. However, there is no general model for coupled systems in which solid deformation and fluid flow occur conjunctively. Depending on the physical nature of the phenomena different mathematical procedures and schemes have been constructed to solve these problems. Generally two different approaches have been proposed for the solution of fluid solid interaction problems [1, 2]. The first approach is to solve the fluid and solid equations separately. The linking of the two phases is achieved by an iterative procedure. The second approach solves the fluid and solid equations simultaneously. The main problem with the first approach is to maintain continuity across the interface between for the direct linking of fluid and solid regimes which resolves the stated problems. the two phases. The second approach suffers from a mathematical difficulty as the governing system of coupled equations may become ill-conditioned. In the present work a novel nodal replacement technique has been developed.

2. GOVERNING MODEL EQUATION USED IN THE WORK

Using a planar two-dimensional coordinate system (x, y) the mathematical model describing fluid flow can be written in terms of the following governing equations.

**Fluid phase**

Continuity equation

$$\nabla \cdot \mathbf{V} = 0$$  \hspace{1cm} (1)

(Conservation of mass for incompressible flows)

Cauchy’s equation of motion

$$\rho \frac{\partial \mathbf{V}}{\partial t} + \rho \mathbf{V} \cdot \nabla \mathbf{V} = \rho \mathbf{g} + \nabla \mathbf{\sigma}$$  \hspace{1cm} (2)

(Conservation of momentum)

where \( \mathbf{V} \) is the velocity field, \( \rho \) is the fluid density and \( \mathbf{g} \) is the body force per unit volume of fluid. For highly viscous fluids such as polymers, the convection term (i.e. \( \mathbf{V} \cdot \nabla \mathbf{V} \)) in equation (2) is usually small and can be neglected. The Cauchy stress is given as

$$\mathbf{\sigma} = -p \delta + \mathbf{\tau}$$  \hspace{1cm} (3)

where \( p \) is hydrostatic pressure, \( \delta \) is unit second-order tensor (kronecker delta) and \( \mathbf{\tau} \) is the extra stress tensor.
Substituting Cauchy stress from equation (3) in equation (2) lead to governing equations for the fluid region [3].

For generalized Newtonian fluids the extra stress tensor in the fluid phase is expressed, explicitly, in terms of rate of deformation as

$$\tau = 2\eta \frac{D}{\partial t}$$  \hspace{1cm} (4)

where $\eta$ and $D$ are viscosity and rate of deformation, respectively.

**Solid phase**

The basic equations of solid deformation in a planar two-dimensional coordinate system ($x$, $y$) dimensional coordinate system ($x$, $y$) are as follows [4]

Equilibrium equations

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{yx}}{\partial x} + \Phi_x = 0$$

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yx}}{\partial y} + \Phi_y = 0$$  \hspace{1cm} (5)

where $\sigma_x$ and $\Phi_i$ are the components of stress tensor and body force per unit volume, respectively.

Hook's law provides the constitutive equation for small strain and displacement in solid materials. This is written as

$$\begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & e \end{bmatrix} \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ 2\varepsilon_{xy} \end{bmatrix}$$  \hspace{1cm} (6)

where $a$, $b$, $c$, $d$, and $e$ are the components of elasticity matrix, and are expressed in terms of constants, $E$ and $v$ i.e. modulus of elasticity and Poisson ratio, respectively.

Substituting the stress term in equation (5) via equation (6) gives

$$- \frac{\partial}{\partial x} (a \frac{\partial u + b \partial v}{\partial y}) - e \frac{\partial}{\partial y} (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) = f_x$$

$$- \frac{\partial}{\partial x} (\frac{\partial u}{\partial y} + d \frac{\partial v}{\partial x}) - e \frac{\partial}{\partial y} (\frac{\partial u}{\partial x} + d \frac{\partial v}{\partial y}) = f_y$$  \hspace{1cm} (7)
G.khodabakhshi, V.Nassehi, L.shojai and R.J.Wakeman

\[
\begin{align*}
t_x &= (a \frac{\partial u}{\partial x} + b \frac{\partial v}{\partial y}) n_x + c(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) n_y \\
t_y &= e(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) n_x + (b \frac{\partial u}{\partial x} + d \frac{\partial v}{\partial y}) n_y
\end{align*}
\]  

(8)

where, for plane stress

\[
\begin{align*}
a &= d = \frac{E}{1-\nu^2} \\
c &= \frac{\nu E}{1-\nu^2} \\
e &= \frac{E}{2(1+\nu)}
\end{align*}
\]  

(9)

and for plane strain

\[
\begin{align*}
a &= d = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \\
b &= \frac{\nu E}{(1+\nu)(1-2\nu)} \\
e &= \frac{E}{2(1+\nu)}
\end{align*}
\]  

(10)

3. MODELLING SCHEME

In this study a Galerkin finite element scheme that combines mathematical robustness with computing economy has been used to discretise the governing equations. To satisfy the stability condition required in the numerical solution of incompressible flows (known as the LBB criterion [5]), the pressure term in equation (2) is expressed as

\[
P = -\lambda' \nabla \cdot V
\]  

(11)

where

\[
\lambda' = \eta \lambda
\]  

(12)

where \( \lambda' \) is a large number called the penalty parameter [6].

The field variable is approximated as

\[
u = \bar{u} = \sum N_j u_j \text{ etc.}
\]  

(13)

where \( u, N_j \) and \( u_j \) are field variable, shape function and nodal values of field variable, respectively.

Discretised forms of fluid and solid equations are derived using the usual finite element procedure [3, 4].
Resultant equations of fluid flow and solid deformation are written as

**Fluid phase**

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
\mu_x \\
\mu_y
\end{bmatrix} =
\begin{bmatrix}
F_1 \\
F_2
\end{bmatrix}
\]  \hspace{1cm} (14)

where

\[
A_{11} = \int_{\Omega} \left[ (\alpha + 2\eta) \frac{\partial N_1}{\partial x} \frac{\partial N_1}{\partial x} + \eta \frac{\partial N_1}{\partial x} \frac{\partial N_1}{\partial y} \right] d\Omega,
\]

\[
A_{12} = \int_{\Omega} \left[ (\alpha + 2\eta) \frac{\partial N_1}{\partial y} \frac{\partial N_2}{\partial x} + \eta \frac{\partial N_1}{\partial y} \frac{\partial N_2}{\partial y} \right] d\Omega,
\]

\[
A_{21} = \int_{\Omega} \left[ (\alpha + 2\eta) \frac{\partial N_2}{\partial x} \frac{\partial N_1}{\partial x} + \eta \frac{\partial N_2}{\partial x} \frac{\partial N_2}{\partial y} \right] d\Omega,
\]

\[
A_{22} = \int_{\Omega} \left[ (\alpha + 2\eta) \frac{\partial N_2}{\partial y} \frac{\partial N_2}{\partial x} + \eta \frac{\partial N_2}{\partial y} \frac{\partial N_2}{\partial y} \right] d\Omega.
\]  \hspace{1cm} (15)

**Solid phase**

\[
[K^{11}] \{u\} + [K^{12}] \{v\} = \{F^1\}
\]

\[
[K^{21}] \{u\} + [K^{22}] \{v\} = \{F^2\}
\]  \hspace{1cm} (17)

where

\[
K_{ij}^{11} = \int_{\Omega} \left( \alpha \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \eta \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \right) dx dy
\]

\[
K_{ij}^{12} = K_{ij}^{21} = \int_{\Omega} \left( \alpha \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial x} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) dx dy
\]

\[
K_{ij}^{22} = \int_{\Omega} \left( \alpha \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} + \eta \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) dx dy
\]  \hspace{1cm} (18)
\[ F_i^1 = \int_{\Omega_x} N_i f_x \, dx \, dy + \oint_{\Gamma} N_i t_x \, ds \]

Similarity in the resultant fluid and solid equations provides a mean for representing a unique set of equations for both regions. This approach has the flexibility to switch the model from fluid analysis to solid deformation. This results in a significant reduction in computational cost. However, this procedure depends on considering the following relationships which relate the penalty parameter in the fluid equation to the Young modulus and Poisson ratio \[7\].

For plane strain
\[ \lambda = \frac{2vE}{(1-2v)} \]  
(20)

For Plane stress
\[ \lambda = \frac{2Ev}{1-v} \]  
(21)

### 3.1 linking of the working equations of flow and solid phase

To couple the different governing equations of solid and fluid phases, the solid phase equations are imposed as the boundary condition for the fluid equations at the interface between the phases. This imposition circumvents the difficulty of matching the unequal line integrals which arise during the discretisation of governing equations of two phases. In the stiffness matrix of fluid elements terms representing the fluid-solid interface are replaced by terms resulting from the discretisation of solid displacement equations. This procedure is illustrated in figure 1.

![Figure 1 schematic representation of linking phases in this work](image)

### 4. COMPUTER SIMULATIONS

Based on the developed scheme a computer code has been written that yields stable and convergent solutions for the governing equations. A rectangular domain has been chosen and discretised into 400 nine nodded \( C^0 \) bi-quadratic finite elements. The following flowchart describes the steps in the modelling of the present problem (Figure 2).
Figure 2 the modelling strategy
(ne is the element number, m is the number of the first element in solid phase).
4.1 Physical data

Shear viscosity in fluid equations is defined by the power-law model as

$$\eta = \eta_0 (\dot{\gamma})^{n-1}$$

(22)

where $\eta_0$ is the consistency coefficient, $\dot{\gamma}$ is the shear rate and $n$ is power-law index. Numerical values of the parameter used in the present work are shown in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>9800 kg m$^{-3}$</td>
</tr>
<tr>
<td>$\eta_0$</td>
<td>88700 kg m$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$E$</td>
<td>2, 20, 200 Mpa</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.19, 0.29, 0.4, 0.499</td>
</tr>
</tbody>
</table>

Table 1 - Numerical values of physical parameters

4.2 Boundary conditions

The inlet velocity is 0.0001 m/s (in $+y$ direction), no-slip boundary condition has been defined for the solid walls in the fluid region. Zero displacement on the side walls in the solid region has been considered.

5. RESULTS AND DISCUSSION

Variation in physical and mechanical parameters in fluid and solid equations lead to different results in deformation of solid media. The effects of increasing the elasticity modulus on deformation of interface between solid and fluid is shown in Figure 3. Figure 4 shows the deformation of solid material at the interface as rheological behaviour of fluid changes due to changes in power-law index. As the power-law index of the fluid flow decreases, its velocity increases. This results in a higher deformation in the solid phase. Therefore, the highest solid deformation occurs when the power-law index of the interacting fluid is less than unity. The velocity profile and displacement are shown in Figure 5. Figure 6 shows the displacement of interface with the variation of poison ratio. As is shown in these figures, the rheological behaviour of the fluid has a significant effect on the deformation of the solid interface. Similarly as the Poisson ratio approaches 0.5, the solid interface becomes less deformed. This is because that for Poisson ratio of 0.5, the solid should behaves as an incompressible medium. As expected using higher modulus of elasticity, a reduction in the deformation of the interface between the solid and fluid phases has been observed.
Figure 3 Solid displacements at the interface with fluid for solid materials with different elasticity modulus.

Figure 4 Solid displacements at solid fluid interface for fluids with different power-law index ($E=200$ MPa).

Figure 5 Velocity and displacement profiles.
Figure 6 Solid displacement at its interface with fluid for solid materials with different poison ratio (E=2 MPa).

6. CONCLUSION

The proposed scheme satisfies the condition for the coupling of the solid deformation and fluid flow equations. Therefore using the developed scheme, Stokes and linear elastic equations are solved conjunctively. Study of the behaviour of solid and fluid reveals that changing rheological behaviour of the fluid has a significant effect on the deformation of the solid section of the domain.

REFERENCES

Choice of appropriate constitutive equations in modelling of injection moulding of rubber

J. Nassehi, G. Khodabakhshi
Chemical Engineering Department, Loughborough University, Loughborough, Leicestershire LE11 3TU, UK

ABSTRACT: Finite element modelling offers a powerful, geometrically flexible and cost effective tool for quantitative analysis of processes such as injection moulding of elastomers. However, accurate and reliable results can only be obtained if the constitutive behaviour of elastomer is represented by an appropriate equation. This study deals with finite element simulation of mould filling process used in manufacture of rubber products under non-isothermal condition. Free surface flow during the filling of a mould is modelled using a scheme based on the Volume of Fluid (VOF) technique. The overall aim of the present study is to quantify the influence of the most important factors that are envisaged to determine the outcome of mould filling process. Thermal effects, wall slip and mould geometry are amongst the factors that their effect on the outcome of mould filling process are considered to be important. In this paper finite element simulation of temperature profiles within a mould is discussed.

INTRODUCTION

The selection of the most appropriate constitutive equation is of paramount importance in the modelling of elastomeric flows. A large number of viscoelastic constitutive models have been developed to describe the rheological behaviour of elastomers. It is, however essential to be aware that none of these models leads to experimentally verifiable predictions for all types of deformations that an elastomer can be subjected during a forming process. Therefore it is necessary to choose a constitutive equation that is deemed to be suitable for a given case. In addition to this general observation there is an un-\volved theoretical problem with conjunctive solution of visco-elastic constitutive equations with thermal energy balance model [1]. On the other hand, simplistic approaches based on the use of the generalized Newtonian constitutive models which provide straightforward schemes for modelling of thermoplastics processing fail to include elastic effects which are detected in visco-elastic flows. To avoid these difficulties many investigators have suggested a compromise based on the use of a heuristic constitutive model which can take into account the influence of shear deformation on the normal stresses within a visco-elastic flow regime. This model can also be very conveniently included in a non-isothermal analysis of visco-elastic flows. The basic form of this model is derived by Crimi- nale-Ericksen-Filbey [2] and is commonly known as the CEF model.

The CEF model is a form of second-order fluid behaviour model which is most suitable for viscometric flows. A viscometric flow is defined as one in which the deformation as seen in a reference frame which translates and rotates with a fluid element is indistinguishable from simple shear [3].

The selection of mould geometry and flow domain characteristics justify the use of viscometric approach in the present simulation.

2. GOVERNING MODEL EQUATIONS USED IN THE PRESENT WORK
Using a two-dimensional coordinate system \((x,y)\), the mathematical model describing flow of an incompressible fluid can be written in terms of following governing equations.

1) Continuity equation (based on mass balance)
   \[ \nabla \cdot \mathbf{V} = 0 \quad (1) \]

2) Cauchy’s equation of motion (based on momentum balance)
   \[ \rho \frac{\partial \mathbf{V}}{\partial t} + \rho \mathbf{V} \cdot \nabla \mathbf{V} = -\nabla P + \nabla \tau \quad (2) \]

where \( \mathbf{V} \) is the velocity field, \( \rho \) is the fluid density, \( \tau \) is the pressure and \( \tau \) is the extra stress tensor.

3) Constitutive model. In the present work the following CEF equation is used.
   \[ \tau = 2\eta D - \Psi_1 D + 4\Psi_2 D^2 \quad (3) \]

where \( \eta \) is the fluid viscosity, \( \Psi_1 \) and \( \Psi_2 \) are the first and second normal stress difference coefficients, respectively, and

\[ \frac{\partial D}{\partial t} = \frac{\omega}{\omega} \cdot D - D \cdot \omega - 2D^2 \quad (4) \]

\( \omega \) is the upper convected time derivative of \( D \), \( \frac{\partial D}{\partial t} \) is the local time derivative (which should be neglected in a viscometric flow). Here \( D = \frac{1}{2}[\nabla \mathbf{V} + (\nabla \mathbf{V})^T] \)

\( \omega = \frac{1}{2}[\nabla \mathbf{V} - (\nabla \mathbf{V})^T] \) is the anti-symmetric part of the rate of deformation (or rate of strain) tensor. Therefore the CEF model relates explicitly the extra stress appearing in the equation of motion to the rate of strain (i.e. rate of deformation) within the fluid. As the rate of strain is defined in terms of velocity gradients this results in the elimination of the stress components from the equation of motion yielding a determinate set of equations which can be solved.

In the present work fluid viscosity is defined using a power-law model. The first and second normal stress differences in a viscometric flow are functions of shear rate. These parameters can be found using empirical relationships [4].

The advancing flow front within the mould is simulated using the VOF (volume of fluid) technique [5]. This method is based on the solution of the surface position probability density equation, given as:

\[ \frac{\partial F}{\partial t} + \mathbf{V} \cdot \nabla F = 0 \quad (5) \]

where \( 0 \leq F \leq 1 \) is called the surface position function.

It is the common practice to maintain the body of moulds at high temperatures to facilitate moulding of elastomers. Nevertheless significant viscous heat dissipation occurs in normal moulding processes and hence it is not realistic to assume that such operations remain isothermal. Therefore in conjunction with the described flow model the following heat balance equation should also be solved to quantify the effects of non-uniform temperature distribution within the mould on the outcome of the process.

\[ \rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q \quad (6) \]

where \( T \) is the temperature field, \( c \) and \( k \) are the heat capacity and thermal conductivity of the elastomer, respectively and \( q \) is the viscous heat dissipation, calculated as viscosity times the square of the shear rate.

3. MODELLING SCHEME

A continuous penalty/Galerkin finite element scheme which combines efficiency with computing economy, has been used in order to solve the above described model equations. In this scheme the pressure in the equation of motion is substituted by

\[ P = -\lambda \nabla \cdot \mathbf{V} \quad (7) \]

where \( \lambda \) is called the penalty parameter. Time stepping is based on the use of well known implicit
method [5]. The cycle consisting of the decoupled computations of field variables (i.e. velocity, free surface position and temperature) is iterated until convergence is achieved. Time variable is then incremented and the cycle is repeated till the predetermined end of simulation. The velocity field obtained using the continuous penalty scheme provides the necessary data for generating the pressure field via the variational recovery method [6]. At the end of each cycle the free surface equation is solved using an up-winded Galerkin scheme. Values of the free surface position function corresponding to the filled, empty and position of the free surface are 1, 0 and 0.5, respectively [7].

Consistent Stream line Upwind Petrov Galerkin scheme is used for solution of energy balance equation [6].

**COMPUTER SIMULATIONS**

The mould to be studied these effects is of two-plate design whose schematic diagram is shown in Figure 1. The feed system for this mould consists of a sprue connected to a U shaped runner, which ends in a diverging gate. The material is injected through the sprue at a constant flow rate using an injector. The injector is a displacement device, which is designed to maintain a steady flow rate entering into the runner through the sprue. The injection continues until the mould is filled.

**4.1 Physical data**

Shear viscosity is defined by the power-law model as

\[ \eta = \eta_0 (\dot{\gamma})^{(n-1)} e^{-b(T-T_{ref})} \]  

where \( \eta_0 \) is consistency coefficient, \( \dot{\gamma} \) is the shear rate, \( n \) is power-law index, \( b \) is temperature dependency coefficient and \( T_{ref} \) is a reference temperature. The first and second normal stress difference coefficients are found using the following empirical relationship [8]:

\[ \Psi_1 = A\dot{\gamma}^2 \]  
\[ \Psi_2 = 0.1\Psi_1 \]  

where \( A \) and \( B \) are experimentally determined characteristic constants of an elastomer. Numerical values of the parameters used in the present work are shown in the following table.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>9800 kg m(^{-3})</td>
</tr>
<tr>
<td>( c )</td>
<td>1255 J kg(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( k )</td>
<td>0.13 W m(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( \eta_0 )</td>
<td>88700 kg m(^{-1}) s(^{-1})</td>
</tr>
<tr>
<td>( b )</td>
<td>0.012 K(^{-1})</td>
</tr>
<tr>
<td>( T_{ref} )</td>
<td>383 K</td>
</tr>
<tr>
<td>( A )</td>
<td>0.00347</td>
</tr>
<tr>
<td>( B )</td>
<td>1.66</td>
</tr>
</tbody>
</table>

**4.2 Initial and Boundary conditions.**

Initial velocity = 0 everywhere. Inlet velocity = 0.1 m s\(^{-1}\) (corresponding to a constant volumetric flow rate) and no slip at solid walls has been assumed. Inlet temperature 450 K, wall temperature 405 K.

**4.3 Data used in the finite element scheme**

Penalty parameter \( \lambda = 10^6 \). Time increment \( \Delta t = 0.01667 \) s. Initially, the flow domain is discretised into 1100 nine node C\(^0\) bi-quadratic finite elements and the convergence of the solutions is checked via mesh refinement by doubling the number of elements after the initial run.

The mould filling operation considered here takes 14.28 s in total. Choosing a time increment of 0.01667 s the process is simulated through nearly 857 steps.

Simulated flow front obtained using Phan-Thanh/Tanner and CEF models are previously published.
and consistency of the model results has been verified [4, 8]. New data obtained solving the energy equation are presented in this paper. Predicted temperature values at various sampling points within he filled sections of the mould chamber are shown in Figure 2. In each selected time step the results are shown in 3 vertical (base, middle, and top of the filled section of the mould) and 5 horizontal positions (equally positions across the mould width at the entrance and middle of the filled part).

As it can be seen the maximum value of temperature is in the middle of the filled section of the mould decreasing as the elastomer approaches the boundaries of the mould.

5. CONCLUSIONS

The developed finite element scheme is shown to generate useful simulations for the mould filling process. CEF model has been employed to take into account both the visco-elastic behaviour of elastomeric fluid and non-isothermal nature of the process. As the computational results indicate there are significant temperature variations within the mould. Such large temperature variations may be reduced to a degree if the temperature at the mould walls kept equal to the temperature of the elastomer at the inlet. However, the elastomer passing through the U shaped runner suffers significant deformation and hence it is not realistic to assume that its temperature will remain equal to its initial value at the inlet. Furthermore the is expected to demonstrate an uneven deformation on its parts during the flow through the U shaped runner.

REFERENCES

Appendix 3

Program Manual

1. Fortran code
2. Input data
3. Output file
The Algebraic equations are solved by the finite element method. Velocity components and pressure are the prime unknowns in the flow field. Concentration in the flow field is also calculated.

A complete list of options is given on the program listing. The program consists of a main module and subroutines. The program is written in PORTTRAN programming language.

MacTsy and Navaraj S. Meenakshi and modified by Goodarz Khodabakhshi for Fluid Solid Interaction systems.

List of Subroutines

work file
*********

file contents

51 input data file
60 output file for documentation
11 output file containing velocity field data for plotting
12 output file containing concentration data for contour plotting
14 used as a work file in the solver routine
15 stores shape functions and their derivatives at 'full' integration points
17 output file containing pressure data for contour plotting
20 output file containing elemental stiffness matrix

List of variables

as (27, 27) element coefficient matrices on LHS X (27, 27) element coefficient matrices on RHS b (27, 9) global derivatives of shape functions bc (maxdf) nodal constraints (boundary conditions) conc (maxxp) nodal concentrations cord (maxxp,minx) nodal coordinates del (27, 9) local derivatives of shape functions vel (maxdf) nodal velocities decl, decs depths of slip layers grav first component of the applied force body grav second component of the applied force body icord indicates whether the coordinate system is cartesian (planar) or cylindrical (axisymmetric) tolcl convergence tolerance factor for concentration tolcp convergence tolerance factor for pressure tolcv convergence tolerance factor for velocities nbc total number of boundary-node constraints ncn number of nodes per element ndf degree of freedom per node ndim dimensions of the solution domain nel total number of elements nint total number of integration points nnp total number of nodal points noda (maxel, 27) element connectivity

maxiter maximum number of iterations for non-newtonian case num max integration points per element press(maxp) nodal pressures r1 (maxdf) global load vector (r.h.s.) rffct friction coefficient (slip) rtr (27) element load vector stiff(maxar) global stiffness matrix (a in a*x=h.s.) rvisc power law index rstep reference temperature rpress reference pressure rpsd power law index rpsd reference temperature rvisc coefficient relating viscosity to temperature rpsd coefficient relating viscosity to pressure rpsd shear rate nwr no. of sample nodes for recording transient solutions

List of variables

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Program Navieruvp

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This is a program for the solution of non-newtonian, non-isothermal, incompressible flow problems using the weighted residual galerkin method.

The solution scheme is based on the U-V-P method. Velocity components and pressure are the prime unknowns in the flow field. Concentration in the flow field is also calculated.

Algebraic equations are solved by a frontal method.

A complete list of options is given on the program listing. The program consists of a main module and subroutines. The program is written in PORTTRAN programming language.

Developed by Walter R. Musiwa and Naraj S. Meenakshi and modified by Goodarz Khodabakhshi for Fluid Solid Interaction systems.

******************************************************************************

work file
*********

file contents

51 input data file
60 output file for documentation
11 output file containing velocity field data for plotting
12 output file containing concentration data for contour plotting
14 used as a work file in the solver routine
15 stores shape functions and their derivatives at 'full' integration points
17 output file containing pressure data for contour plotting
20 output file containing elemental stiffness matrix

List of variables

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maxiter maximum number of iterations for non-newtonian case num max integration points per element press(maxp) nodal pressures r1 (maxdf) global load vector (r.h.s.) rffct friction coefficient (slip) rtr (27) element load vector stiff(maxar) global stiffness matrix (a in a*x=h.s.) rvisc power law index rstep reference temperature rpress reference pressure rpsd power law index rpsd reference temperature rvisc coefficient relating viscosity to temperature rpsd coefficient relating viscosity to pressure rpsd shear rate nwr no. of sample nodes for recording transient solutions

******************************************************************************

List of Subroutines

******************************************************************************

backsub backsubstitution method for finding the final solution vector
clean cleans the arrays and prepares them for solution
cncg calculates the concentrations
cntol makes a check for the convergence
cderv calculates the jacobian matrix, its determinant and global derivatives of the shape functions
cflow calculates the velocities and pressures
cfront frontal method for solving the final set of equations
gaussp specifies the gauss points and weights for quadrature integration
gbc Calculates the primary boundary conditions
geval specifies the nodal connectivity array
ggetd Reads the input material data
ggeto reads the modal connectivity data
ggetn Creates the modal connectivity array
g5mp evaluates the terms of the mass matrix
ghome imposes the primary boundary conditions for velocity
ghpbc imposes the primary boundary conditions for concentration
ghsetm Sets the location data for nodal degrees of freedom
ghshape calculates the shape functions and their derivatives
ghslip identifies the upper and lower boundary layers
ghstress calculates stress components at integration points
ghvisc Calculates the viscosity
ghvisc Calculates virtual viscosity for wall flows

******************************************************************************

storage allocation

******************************************************************************

dimension title (80)
dimension node (maxel, 27), nmax (maxel, 9), ncord (maxp, 2)
dimension node (maxdf), nbc (maxdf), ncn (maxdf), ndf (maxdf), ndim (maxdf)
dimension vel (maxdf), vcon (maxdf), vpress (maxdf)
dimension r1 (maxdf), rl (maxdf), rtr (27)
dimension clmp (maxp), stemp (maxp), stemp (maxp), stemp (maxp), stemp (maxp), stemp (maxp)
dimension vnp (maxdf)
dimension as (maxst,maxst)
Read input data from main data file and prepare arrays for solution process

```
call gmat (mel, nmat, pmat, 51, 60, maxel, rtem)
spef

call gnod (mp, corg, 51, 60, maxnp, ndim, icord)
call gelm (mel, ncn, node, 51, 60, maxel)
call gbedh (nbc, iibc, jibc, vbc, 51, 60, maxnc)
```

Set control parameters (default values are overwritten by input data if specified)

```
cnnc number of nodes per element
ngaus number of integration points
nter maximum number of iterations for non-newtonian case
ndim number of space dimensions in the solution domain
```

```
cd 5125 iel = 1, maxel
5125 continue
```

```
call flow (node, corg, pmat, nopp, nelf, ndf, ndm)
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call seircv
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```
c thetas indicates the choice of method being employed in the
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defter maximum number of time steps being employed for finding solution
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A two dimensional finite element model of a...
del(1,1)=0.25*(1-xi)*(1-eta)
del(1,2)=0.25*(1-xi)*(1-eta)
del(2,1)=0.25*(1-xi)*(1-eta)
del(2,2)=0.25*(1-xi)*(1-eta)
p(1)=0.25*(1-xi)*(1-eta)
p(2)=0.25*(1-xi)*(1-eta)
p(3)=0.25*(1-xi)*(1-eta)
p(4)=0.25*(1-xi)*(1-eta)
p(5)=0.25*(1-xi)*(1-eta)
p(6)=0.25*(1-xi)*(1-eta)
p(7)=0.25*(1-xi)*(1-eta)
p(8)=0.25*(1-xi)*(1-eta)
p(9)=0.25*(1-xi)*(1-eta)

eji(1,1)=cj(2,2) detj
eji(2,2)
cji(1,2)=-ej(1,2) detj
cji(2,2)
del(1,1)=cj(1,1) detj
del(1,2)=cj(1,2) detj
del(2,1)=cj(2,1) detj
del(2,2)=cj(2,2) detj
del(k,l)=gash

del(1,1)=-0.25*(1-xi)*(1-eta)
del(1,2)=-0.25*(1-xi)*(1-eta)
del(2,1)=-0.25*(1-xi)*(1-eta)
del(2,2)=-0.25*(1-xi)*(1-eta)
p(1)=-0.25*(1-xi)*(1-eta)
p(2)=-0.25*(1-xi)*(1-eta)
p(3)=-0.25*(1-xi)*(1-eta)
p(4)=-0.25*(1-xi)*(1-eta)
p(5)=-0.25*(1-xi)*(1-eta)
p(6)=-0.25*(1-xi)*(1-eta)
p(7)=-0.25*(1-xi)*(1-eta)
p(8)=-0.25*(1-xi)*(1-eta)
p(9)=-0.25*(1-xi)*(1-eta)

eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(1,1)
del(1,2)
del(2,1)
del(2,2)
eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(k,l)
gash

del(1,1)=-0.25*xi*(1-eta)
del(1,2)=-0.25*xi*(1-eta)
del(2,1)=-0.25*xi*(1-eta)
del(2,2)=-0.25*xi*(1-eta)
p(1)=-0.25*xi*(1-eta)
p(2)=-0.25*xi*(1-eta)
p(3)=-0.25*xi*(1-eta)
p(4)=-0.25*xi*(1-eta)
p(5)=-0.25*xi*(1-eta)
p(6)=-0.25*xi*(1-eta)
p(7)=-0.25*xi*(1-eta)
p(8)=-0.25*xi*(1-eta)
p(9)=-0.25*xi*(1-eta)

eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(1,1)
del(1,2)
del(2,1)
del(2,2)
eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(k,l)
gash

del(1,1)=0.25*(2*xi+l)*(1-eta)
del(1,2)=0.25*(2*xi+l)*(1-eta)
del(2,1)=0.25*(2*xi+l)*(1-eta)
del(2,2)=0.25*(2*xi+l)*(1-eta)
p(1)=0.25*(2*xi+l)*(1-eta)
p(2)=0.25*(2*xi+l)*(1-eta)
p(3)=0.25*(2*xi+l)*(1-eta)
p(4)=0.25*(2*xi+l)*(1-eta)
p(5)=0.25*(2*xi+l)*(1-eta)
p(6)=0.25*(2*xi+l)*(1-eta)
p(7)=0.25*(2*xi+l)*(1-eta)
p(8)=0.25*(2*xi+l)*(1-eta)
p(9)=0.25*(2*xi+l)*(1-eta)

eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(1,1)
del(1,2)
del(2,1)
del(2,2)
eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(k,l)
gash

del(1,1)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
del(1,2)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
del(2,1)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
del(2,2)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(1)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(2)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(3)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(4)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(5)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(6)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(7)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(8)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)
p(9)=0.5*xi*0.5*xi*eta+0.25*(eta**2-eta)

eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(1,1)
del(1,2)
del(2,1)
del(2,2)
eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(k,l)
gash

del(1,1)=-0.25*xi*(1-eta)
del(1,2)=-0.25*xi*(1-eta)
del(2,1)=-0.25*xi*(1-eta)
del(2,2)=-0.25*xi*(1-eta)
p(1)=-0.25*xi*(1-eta)
p(2)=-0.25*xi*(1-eta)
p(3)=-0.25*xi*(1-eta)
p(4)=-0.25*xi*(1-eta)
p(5)=-0.25*xi*(1-eta)
p(6)=-0.25*xi*(1-eta)
p(7)=-0.25*xi*(1-eta)
p(8)=-0.25*xi*(1-eta)
p(9)=-0.25*xi*(1-eta)

eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(1,1)
del(1,2)
del(2,1)
del(2,2)
eji(1,1)
eji(2,2)
cji(1,2)
cji(2,2)
del(k,l)
gash

end subroutine deriv
narg = maxfr - 10
if (ielt.eq.1) neli = 0
if (ielt.eq.1) ntrc = 1
if (ntrc.eq.0) goto 6040
maxx = maxfr
ntrc = 0
nerror = 20
lfrom = 0
narg = nmax - 10

1) Find last appearance of each node
==========================================

nlast = 0
do 6030 i = 1, ntrc
do 6020 n = 1, nmax
jdn = ndn(n)
do 6030 l = 1, jdn
if (nop(n, l).eq.1) goto 6030
nlast = n
nlast = n
nlast = n

6030 continue

2) continue
if (nlast.eq.0) goto 6010
nop(nlast, 11) = -nop(nlast, 11)
nlast = 0

6010 continue
ntrix = jdn

3) Assembly
==========================================

4040 continue
if (ielt.gt.1) go to 6060
lcol = 0
do 6050 j = 1, nmax
do 6050 j = 1, nmax
if (j.eq.0) goto 6050

6050 continue

4060 neli = neli + 1
n = neli
jdn = ndn(n)
k = 0
do 6070 j = 1, jdn
nn = nop(n, j)
m = labs(m)
l = nccp(n)
lj = lrj(m)
do 6070 j = 1, lidi
kc = kcol
li = k + 1
if (m.l0li) li = -li
nk(hc) = li

6070 continue

4) Set up heading vectors
==========================================

do 6080 l = 1, lkc
node = nk(lk)
if (lcol.eq.0) goto 6100
do 6090 l = 1, lcol
if (labs(node).eq.labs(lhed(lk))) goto 6110

6090 continue

6100 lcol = lcol + 1
ldest(lk) = lcol
lhed(lcol) = node
go to 6080

6110 ldest(lk) = li
lhed(li) = node

6080 continue

if (lcol.ne.maxx) go to 6130

6130 continue

do 6140 l = 1, lkc
li = ldest(lk)
do 6140 l = 1, lkc
kk = ldest(k)
eq(kk, li) = eq(kk, li) + eq(kk, li) + eq(kk, li) + eq(kk, li)

6140 continue

if (lcol.gt.nerrit.and.ncol.lc) return

6150 lcr = 0
lcr = 0
lcr = 0

lfron = 0
lfron = 0
lfron = 0

1lfrom = 0

if (lfron.eq.0) goto 6160

6160 continue

5) Modify equations with applied boundary conditions
==========================================

6170 continue

if (ir.eq.0) goto 6190

6180 continue

6190 continue

if (lcol.eq.0) go to 6200

6200 continue

6) Search for absolute pivot
==========================================

7) Normalize pivotal row
==========================================

8) Eliminate then delete pivotal row and column
==========================================
lpivc = lpivo+1
do 6260 1 = 1,lpivo
eq(k,1) = eq(k,1)-fac*qq(1)
6260 continue
if(lpivc.eq.icol(1)) go to 6290
lpivc = lpivo+1
do 6260 1 = 1,lpivo
eq(k,1) = eq(k,1)-fac*qq(1)
6260 continue
rpivc = r(kw)-fac*rhs
c6290 continue
if(lpivc.eq.icol(1)) go to 6310
lpivc = kpivro
6310 k = kpivro,icol
kw = iabs(icol(1))
fac = eq(k,1),pivco
pivko(k) = fac
if(lpivc.eq.icol(1)) go to 6330
lpivc = kpivro
6330 if(lpivc.eq.icol(1)) go to 6350
lpivc = kpivro
do 6320 1 = 1,icol
eq(k,1) = eq(k,1)-fac*qq(1)
6320 continue
if(lpivc.eq.icol(1)) go to 6350
lpivc = kpivro
6350 rw(k) = r(kw)-fac*rhs
c6360 continue
continue
continue
Write pivotal equation on dispatcher
print(9990,48) rw(kw),r(kw),pivko(k)
continue
continue
Rearrange heading vectors
icol = icol-1
if(lpivc.eq.icol+l) go to 6370
do 6380 1 = 1,icol
eq(1,icol) = 0
eq(icol,1) = 0
6370 continue
if(icol.eq.icol) return
do 6380 1 = 1,icol
eq(1,icol) = 0
eq(icol,1) = 0
6380 continue
continue
continue
Determine whether to assemble,eliminate or back substitute
if(icol.gt.ncrit) go to 6510
if(ifix(ipos).ne.0) return
if(icif(icol).ne.icol) return
do 6380 1 = 1,icol
eq(1,icol) = 0
eq(icol,1) = 0
6380 continue
continue
continue
do 6410 if(abs(pivot).lt.1d-28) go to 6410
c6410 continue
rpivc = r(kw)/pivko
write(ntot,1404)icol,rpivc,icol
continue
continue
call baesub
1 (ntov, ncmd, bc, r1, vel, press, 2 maxfr, qq, lhed, ncl)
c main exit with solution
continue
continue
0
solv
1 (moda, coord, post, napp, nfd, xdn,
2 ncmd, bc, vel, press, r1, temp,
3 ldest, kdest, nk, eq, lhed, bhed,
4 k piv, kpiv, jsad, qq, pivko, itct,
5 nol, nqes, pagw, pagw,
6 gravx, p, del, b dirse, navel,
7 maxpe, maxfr, maxfr, maxfr,
8 xg, da, rto, icoord, rr, le,
9 deltax, theta, 4dv, sinv, exp, velcound)
implicit double precision(a-h,o-z)

dimension node (maxel,maxst),pmat(maxel),9.cord (maxnp,ndia)
dimension nco0 (maxdf),bc (maxdf),.sin (maxaxl, nc)</dimension
dimension vel (nnp, ndia,zi (maxd),conc (maxnp)
dimension as (maxaxl,maxst),rz (maxst)
dimension xg (3,icj)
dimension x (2,ik)
dimension pbnc (2,ibh (2,ik)
dimension p (9,del (2,ik (2,9),b (2,ik (2,9)
dimension eq (maxfr, maxst),mopp (maxdf)
dimension idse (22)
dimension lndse (maxfr),lbed (maxfr),bbed (maxfr)
ndmod (maxfr)
dimension pnv (maxfr),kpv (maxfr)
ndq (maxfr)
dimension pnv0l(maxfr),mdf (maxdf)
ndn (maxdf)
dimension ppp (9,pp (9,pp (9,pp

dimension ak (maxaxl,maxst),akf (maxst)
dimension press (maxnp,2,9,trimaxp)
dimension gdf (2,ik,9,temp)
dimension dmass (maxaxl,maxst)
dimension a00l (maxaxl, maxst)
dimension a02 (maxaxl,maxst)
dimension a00l (maxaxl, maxst)
dimension a02 (maxaxl,maxst)
dimension a00l (maxaxl, maxst)
dimension a02 (maxaxl,maxst)

dimension rvisc = pmct(iel,1)
rpef = pmct(iel,1)
power = pmct(iel,1)
ttem = pmct(iel,1)
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tem = pmct(iel,1)
tem = pmct(iel,1)
tem = pmct(iel,1)
tem = pmct(iel,1)
write (15) iel,iig,jif,jif,del,b,da
else
if (.not. eof (15)) unread (15) iel,iig,jif,jif,del,b,da
endif

calculation of viscosity based on the constitutive equation

--- Stiffness Matrix of Left Hand Side ---

For Transient state (Carnelian co-ordinate system)

aa(j1,j2) = aa(j1,j2) + p[i] * p[j] * da
1 + 0.1*theta*delta*delta*
2 velsound = velsound*b(1,i)*b(1,j)*da
3 + (theta*2.0*visc*b(1,i)*b(1,j)*

--- Stiffness Matrix of Left Hand Side ---

For Transient state (Carnelian co-ordinate system)

aa(j1,j2) = aa(j1,j2) + p[i] * p[j] * da
1 + 0.1*theta*delta*delta*
\[
\begin{align*}
\text{ak}(j_{11}, j_{21}) &= \text{ak}(j_{11}, j_{21}) + (1.0 - \text{theta}) \times \text{theta} \times (c_{11} \times b(1, i) \times b(1, j) + c_{66} \times b(2, i) \times b(2, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{11}, j_{22}) &= \text{ak}(j_{11}, j_{22}) + (1.0 - \text{theta}) \times (c_{12} \times b(1, i) \times b(2, j) + c_{66} \times b(2, i) \times b(1, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{11}, j_{23}) &= \text{ak}(j_{11}, j_{23}) + (1.0 - \text{theta}) \times \text{theta} \times (c_{22} \times b(2, j) + c_{66} \times b(1, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{12}, j_{21}) &= \text{ak}(j_{12}, j_{21}) + (1.0 - \text{theta}) \times (c_{12} \times b(1, j) \times b(2, i)) \\
&\quad \times \text{da} \\
\text{ak}(j_{12}, j_{22}) &= \text{ak}(j_{12}, j_{22}) + (1.0 - \text{theta}) \times (c_{66} \times b(1, j) \times b(2, i)) \\
&\quad \times \text{da} \\
\text{ak}(j_{12}, j_{23}) &= \text{ak}(j_{12}, j_{23}) + (1.0 - \text{theta}) \times \text{theta} \times (c_{22} \times b(2, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{13}, j_{21}) &= \text{ak}(j_{13}, j_{21}) + (1.0 - \text{theta}) \times (c_{66} \times b(1, i) \times b(1, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{13}, j_{22}) &= \text{ak}(j_{13}, j_{22}) + (1.0 - \text{theta}) \times (c_{66} \times b(2, i) \times b(2, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{13}, j_{23}) &= \text{ak}(j_{13}, j_{23}) + (1.0 - \text{theta}) \times \text{theta} \times (c_{22} \times b(2, i)) \\
&\quad \times \text{da} \\
\text{ak}(j_{13}, j_{24}) &= \text{ak}(j_{13}, j_{24}) + (1.0 - \text{theta}) \times (c_{66} \times b(1, i) \times b(2, j)) \\
&\quad \times \text{da} \\
\text{ak}(j_{13}, j_{25}) &= \text{ak}(j_{13}, j_{25}) + (1.0 - \text{theta}) \times (c_{66} \times b(2, i) \times b(1, j)) \\
&\quad \times \text{da} \\
\end{align*}
\]
\[ a_k(j_{11}, j_{22}) = a_k(j_{11}, j_{22}) + (1 - \theta) a_k(j_{11}, j_{22}) \]
\[ (1 - \theta) b(j_{11}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{21}) = a_k(j_{12}, j_{21}) + (1 - \theta) a_k(j_{12}, j_{21}) \]
\[ (1 - \theta) b(j_{12}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{21}) = a_k(j_{13}, j_{21}) + (1 - \theta) a_k(j_{13}, j_{21}) \]
\[ (1 - \theta) b(j_{13}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{22}) = a_k(j_{12}, j_{22}) + (1 - \theta) a_k(j_{12}, j_{22}) \]
\[ (1 - \theta) b(j_{12}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{22}) = a_k(j_{13}, j_{22}) + (1 - \theta) a_k(j_{13}, j_{22}) \]
\[ (1 - \theta) b(j_{13}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{23}) = a_k(j_{12}, j_{23}) + (1 - \theta) a_k(j_{12}, j_{23}) \]
\[ (1 - \theta) b(j_{12}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{21}) = a_k(j_{12}, j_{21}) + (1 - \theta) a_k(j_{12}, j_{21}) \]
\[ (1 - \theta) b(j_{12}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{21}) = a_k(j_{13}, j_{21}) + (1 - \theta) a_k(j_{13}, j_{21}) \]
\[ (1 - \theta) b(j_{13}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{22}) = a_k(j_{12}, j_{22}) + (1 - \theta) a_k(j_{12}, j_{22}) \]
\[ (1 - \theta) b(j_{12}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{22}) = a_k(j_{13}, j_{22}) + (1 - \theta) a_k(j_{13}, j_{22}) \]
\[ (1 - \theta) b(j_{13}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{23}) = a_k(j_{12}, j_{23}) + (1 - \theta) a_k(j_{12}, j_{23}) \]
\[ (1 - \theta) b(j_{12}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{21}) = a_k(j_{13}, j_{21}) + (1 - \theta) a_k(j_{13}, j_{21}) \]
\[ (1 - \theta) b(j_{13}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{22}) = a_k(j_{12}, j_{22}) + (1 - \theta) a_k(j_{12}, j_{22}) \]
\[ (1 - \theta) b(j_{12}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{22}) = a_k(j_{13}, j_{22}) + (1 - \theta) a_k(j_{13}, j_{22}) \]
\[ (1 - \theta) b(j_{13}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{23}) = a_k(j_{12}, j_{23}) + (1 - \theta) a_k(j_{12}, j_{23}) \]
\[ (1 - \theta) b(j_{12}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{21}) = a_k(j_{13}, j_{21}) + (1 - \theta) a_k(j_{13}, j_{21}) \]
\[ (1 - \theta) b(j_{13}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{22}) = a_k(j_{12}, j_{22}) + (1 - \theta) a_k(j_{12}, j_{22}) \]
\[ (1 - \theta) b(j_{12}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{22}) = a_k(j_{13}, j_{22}) + (1 - \theta) a_k(j_{13}, j_{22}) \]
\[ (1 - \theta) b(j_{13}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{23}) = a_k(j_{12}, j_{23}) + (1 - \theta) a_k(j_{12}, j_{23}) \]
\[ (1 - \theta) b(j_{12}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{21}) = a_k(j_{13}, j_{21}) + (1 - \theta) a_k(j_{13}, j_{21}) \]
\[ (1 - \theta) b(j_{13}, j_{21}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{22}) = a_k(j_{12}, j_{22}) + (1 - \theta) a_k(j_{12}, j_{22}) \]
\[ (1 - \theta) b(j_{12}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{22}) = a_k(j_{13}, j_{22}) + (1 - \theta) a_k(j_{13}, j_{22}) \]
\[ (1 - \theta) b(j_{13}, j_{22}) \cdot \frac{d}{da} \]

\[ a_k(j_{13}, j_{23}) = a_k(j_{13}, j_{23}) + (1 - \theta) a_k(j_{13}, j_{23}) \]
\[ (1 - \theta) b(j_{13}, j_{23}) \cdot \frac{d}{da} \]

\[ a_k(j_{12}, j_{23}) = a_k(j_{12}, j_{23}) + (1 - \theta) a_k(j_{12}, j_{23}) \]
\[ (1 - \theta) b(j_{12}, j_{23}) \cdot \frac{d}{da} \]
**Stiffness Matrix of Left Hand Side**

\[ \text{akOl} (j13, j23) = \text{akOl} (j13, j22) = \text{akOl} (j13, j21) \]

\[ \text{akOl} (j12, j23) = \text{akOl} (j12, j22) = \text{akOl} (j12, j21) \]

\[ \text{akOl} (j11, j23) = \text{akOl} (j11, j22) = \text{akOl} (j11, j21) \]

\[ \text{aaOl} (j13, j22) = \text{aaOl} (j13, j21) = \text{aaOl} (j13, j20) \]

\[ \text{aaOl} (j12, j22) = \text{aaOl} (j12, j21) = \text{aaOl} (j12, j20) \]

\[ \text{aaOl} (j11, j22) = \text{aaOl} (j11, j21) = \text{aaOl} (j11, j20) \]

**Term one on RHS**

\[ \text{velsound} \cdot \text{velsound} \cdot \text{b}(2,i) \cdot \text{b}(2,j) \cdot \text{da} \]

\[ \text{velsound} \cdot \text{velsound} \cdot \text{b}(1,i) \cdot \text{b}(2,j) \cdot \text{da} \]

\[ \text{velsound} \cdot \text{velsound} \cdot \text{b}(2,i) \cdot \text{b}(1,j) \cdot \text{da} \]

\[ \text{velsound} \cdot \text{velsound} \cdot \text{b}(1,i) \cdot \text{b}(1,j) \cdot \text{da} \]

**For Transient State (Cartesian Co-ordinate System)**

\[ \text{if (i1.eq.20) then} \]

\[ \text{end if} \]

\[ \text{end if} \]

\[ \text{end if} \]

\[ \text{end if} \]
do 7000 i=1,ncn
   jl1 = i
   jl2 = i + ncn
   jl3 = i + 2*ncn
   nn = iabs(node(iel, jl1))
   akf(jl1) = akf(jl1) + ak(jl1, jl2)*vel(nn, 1) + ak(jl1, jl3)*press(nn),
   akf(jl2) = akf(jl2) + ak(jl1, jl2)*vel(nn, 1) + ak(jl2, jl3)*press(nn),
   akf(jl3) = akf(jl3) + ak(jl1, jl2)*vel(nn, 1) + ak(jl2, jl3)*press(nn),
   continue
7000 continue

c Evaluation of Elemental Load Vector
=========================================

do 6085 i=1,ncn
   jl1 = i
   jl2 = i + ncn
   jl3 = i + 2*ncn
   rr(jl1) = akf(jl1),
   rr(jl2) = akf(jl2),
   rr(jl3) = akf(jl3),
6085 continue

For Transient State (Cartesian Co-ordinate System)

rr(jl1) = akf(jl1),
rr(jl2) = akf(jl2),
rr(jl3) = akf(jl3),
6085 continue

maxelm=mxsd

call front
1 (aa, rr, ile, node, maxel, maxst, 2
   ndst, kdst, nk, maxr, eq, lind, 3
   knod, kpiv, lpiv, jmod, qf, psvol, 4
   vel, rl, ncod, bc, nopp, sdf,
5
   ndn, maxdf, nel, maxte, ntev, lcol,
6
   nel1, ntra, press )
return
end

subroutine stress
1 (nel, ncn, node, b, vel, maxnp, maxel, maxst, rvisc )

c implicit double precision(a-h,o-z)
2
c arguments
3
c non number of nodes per element
4
c node array for element connectivity data
5
c dev1 input device id.
6
c dev2 output device id.
7
c maxel see below
8
c dimension node (maxel, ncn)
9
do 5000 iel = 1, nel

c ui1 = 0.0
10
c ui2 = 0.0
11
c u12 = 0.0
12
do 6020 icn = 1, ncn
   jcn = iabs(node(iel, icn))
4020 continue

c
c cartesian components of the stress tensor
==========================================

c ud11 = 2.0 * rvisc * u11
ud12 = rvisc * (u12 + u11)
ud22 = 2.0 * rvisc * u12,

c 5000 continue

c return
end
C subroutine getbc (nbc , ibc , jbc , vbc: idvl, idv2, maxbc)
C arguments
  nbc number of nodal constraint data
  ibc array for constrained nodal points
  jbc array for constrained degree of freedom
  vbc array for boundary values
  idvl input device id.
  idv2 output device id.
  maxbc see below
C
if (.not. eof(51)) read (idv1,1010) (ibc(ind),jbc(ind),vbc(ind))
  (ind=1,nbc)
C print, * boundary conditions array read
write(idv2,3010)
  (ibc(ind),jbc(ind),vbc(ind))
  (ind=1,nbc)
C return
C subroutine putbcv
C arguments
  nbc, nbe, ncod, maxbc, vbc, ntrix
C implicit double precision (a-h.o-s)
C
C arguments
  ncod array for constraint switch defined for every d.o.f.
  vbc array for storing constraint value
  maxbc see below
C ntrix see below
C
dimension ibc (maxbc), jbc (maxbc), vbc (maxbc)
C dimension ncod (maxdf), be (maxdf)
C do 6010 ind = 1, nbc
C if (ibc(ind) .ne. 0) goto 6010
C ntrix = ntrix + ncod(ind) + 1
C ncod(ind) = 1
C return
C subroutine setprm
C arguments
  nmp, nbc, ibc, jbc, vbc, ntrix, ncod, maxbc
C implicit double precision (a-h.o-s)
C
C arguments
  nmp array for constraint switch defined for every d.o.f.
  ibc array for storing constraint value
  jbc array for constrained degree of freedom
  vbc array for constrained nodal points
  ntrix array for constrained nodal points
  ncod array for constrained nodal points
  maxbc see below
C
dimension iibc (maxbc), jibc (maxbc), vbc (maxbc)
C dimension ibe (maxbe), vbe (maxbe)
C do 6010 ind = 1, nbe
C if (ibc(ind) .ne. 0) goto 6010
C ibe(ind) = ibc(ind) + (jbc(ind) - 1) * nmp
C vbe(ind) = vbc(ind)
C return
C subroutine settrix
C arguments
  ntrix, ncod, maxdf
C implicit double precision (a-h.o-s)
C
C argument same as subroutine putbcv
C dimension ibc (maxbc), jbc (maxbc), vbc (maxbc)
C dimension ncod (maxdf), be (maxdf)
C do 6010 ind = 1, nbc
if (ibc(ind).eq.3) then
jnd = ibc(ind)
ncod(ind) = 1
endif
6010 continue
C return
C subroutine setnmp
C arguments
  nmp, nbe, ncod, maxdf
C implicit double precision (a-h.o-s)
C
C arguments
  nmp array for constraint switch defined for every d.o.f.
  nbe array for storing constraint value
  ncod array for constrained nodal points
  maxdf see below
C
dimension iibc (maxbc), jibc (maxbc), vbc (maxbc)
C dimension ibe (maxbe), vbe (maxbe)
C do 6010 ind = 1, nbe
C if (ibc(ind) .ne. 0) goto 6010
C ibe(ind) = ibc(ind) + (jbc(ind) - 1) * nmp
C vbe(ind) = vbc(ind)
C return
C subroutine setntrix
C arguments
  ntrix, ndn, nopp, node, maxdf
C implicit double precision (a-h.o-s)
C
C arguments
  ntrix array of element connectivity
  ndn array of nodal constraint
  nopp array of nodal constraint
  maxbe see below
  maxdf see below
C
dimension node (maxel,maxst), ndn (maxdf) ,nopp (maxdf)
C do 6010 iel = 1, maxel
C write(11,2010) (node(iel,ind), ndn(iel,ind))
C if (ndn(iel,ind) .ne. 1) then
C nopp(iel,ind) = 1
C endif
C return
C subroutine write
C arguments
  idvl, idv2, idv3, idv4, idv5, idv6
C implicit double precision (a-h.o-s)
C
C arguments
  idvl input device id.
  idv2 output device id.
  idv3 input device id.
  idv4 output device id.
  idv5 output device id.
  idv6 output device id.
C
C return
subroutine getmat (ne1, nmat, vet, pet)
  implicit double precision(a-h,o-z)
  nmat number of materials
  pmat array for material constants for each element
  idvl input device id.
  idv2 output device id.
  maxel see below
dimension pmat(maxel,9)
write(idv2,3010)
do
  imat = 1 ,nmat
  rvisc, power, tref, tbco, taco.
disp, pref, roden, gamad
print*, 'material properties read'
if(rvisc .eq.0) rvisc = 0.0
if(pref .eq.0) pref = 0.0
do 6020 iel = ifrom ,ito
pmat(iel,1) = rvisc
pamat(iel,2) = pref
pamat(iel,3) = power
pamat(iel,4) = tref
pamat(iel,5) = tbco
pamat(iel,6) = taco
pamat(iel,7) = disp
pamat(iel,8) = roden
pamat(iel,9) = gamad
rvisc = pref
data = tref
1010 continue
return
end

subroutine control (vel, conc, iter, maxdf, errov, errop)
  implicit double precision(a-h,o-z)
  argume ts are already defined
dimension vel (maxdf),conc (maxnp), press (maxnp)
dimension vet (maxdf),cet (maxnp) , pet (maxnp)
errv = 0.0
tov = 0.0
errc = 0.0
torc = 0.0
errp = 0.0
torp = 0.0
calculate difference between velocities in consecutive iterations
calculate difference between pressures in consecutive iterations
return
end

subroutine output (nnp, vel, press, maxdf, maxnp, icord)
  implicit double precision(a-h,o-z)
  arguments are already defined
dimension vel(maxdf), press (maxnp), conc(maxnp)
dimension pmat(maxel, 9), actpress(maxnp), cord(maxnp,2)
return
end

1010 format(9d10.5)
write(60,3010)
if(icord.eq.0) write(60,3020)
if(icord.eq.1) write(60,3030)
roden=pmat(I,8)
do 6010 inp=inp+1
actpress(inp)=roden*press(inp)
write(60,3040)inp,vel(inp),vel(nnp),actpress(inp)
c if(inp.ge.4224) then
c cord(inp,1)=cord(inp,1)+vel(inp)
c cord(inp,2)=cord(inp,2)+vel(nnp)
c write(60,3041) inp,cord(inp,1),cord(inp,2)
c end if
6010 continue
format(' nodal velocities and pressures '/)
format(1d.ux uy press'!)
format(1d.ux uy press'!)
format(15,2e13.8)
c3041 format(15,2e20.8)
1040 format(15,2e13.4,2e2.8)
c3041 format(15,2e20.8)
1045 format(':node no. node no. max ux node no. min uy'/)
1050 format(15,2e2.8,15,2e2.8)
1055 format(':node no. node no. max uy node no. min uy'/)
1060 format(15,2e2.8,15,2e2.8)
1065 format(':node no. node no. max p node no. min p'/)
1070 format(15,2e2.8,15,2e2.8)
return
end
subroutine visca
1 (rvisc,power,visc,taco,stem,tcco,spress,pref,tcco,gsad)
2 imp
c implicit double precision(a-h,o-z)
visc = rvisc*((4*gsad)**(power-1.0)/2)
end
subroutine minimax
1 cmax, pmax, vel, conc, press, maxnp, nnp
2 nc, np, nm, ncn, ncm, nvm, nym, nvl
3 nyl, pmin, cmin, vymax, vmin, vymax, vmin
4 ndim, maxdf, actpress
5 implicit real*8 (a-h,o-z)
c dimension conc (maxnp), vel (maxdf)
c dimension press (maxnp)
c dimension actpress (maxnp)
vmax = vel(1)
vmin = vel(1)
vmax = vel(nnp+1)
vmin = vel(nnp+1)
pmax = actpress(1)
pmin = actpress(1)
c if(nm.ge.1) then
c ci = conc(i)
c pm = actpress(i)
pvmax = vel(i)
pvmin = vel(i)
pvmax = vel(nnp+i)
pvmin = vel(nnp+i)
c endif
if (pm.gt.pmax) then
pmax=pm
np =i
endif
c endif
if (ci lt pmin) then
pmin = pi
nm =i
endif
c endif
if (pvmax.gt.vxmax) then
vymax= vmax
nvym =i
endif
c endif
if (pvmax.gt.vymax) then
vymax= vmax
nvym =i
endif
c endif
if (pvmin lt vxmin) then
vxmin = vmin
nvxl =i
endif
c endif
if (pvmin lt vymin) then
vymin = vmin
nvyl =i
endif
c endif
6020 continue
return
end
subroutine secinv
1 (nel, nnp, maxdf, maxel, ncn, b, maxst, node, siv)
2 imp
c calculates the second invariant of rate of deformation
tensor at integration points.
c implicit double precision(a-h,o-z)
c function
---
c calculates the second invariant of rate of deformation
tensor at integration points.
c implicit double precision(a-h,o-z)
do 5000 iel = 1 , nel
   1.0
5010 jg = 1 , ngaus
5010 jg = 1 + ig
if (not. eof(15)) read (15) iiel,iig,jjg,p,del,b,da
   .19+1
do 5020 icn = 1 , ncn
   jcn = jabs(node(iel,icn))
   ncn = jcn + nnp
   do 5020 continue
5000 continue
compute the magnitude of the resultant velocity
do 1::i,nnp
   j = i
   vlfI(j) = sqrt((vel(j,1)**2) + (vel(j,2)**2))
end do
write(603,1000)
write(603,2000) nnp, nnel
dolen=pmat(l,8)
do 1::i,nnp
   j = i
   actpress(j) = dolen*press(j)
write(603,5000) cord(j,1), cord(j,2), vel(j,1), vel(j,2), vlfI(j), actpress(j)
end do
return
end subroutine cosmos
1 (nnp , vel , press , maxdf , maxnp , icord , 2 pmat , maxel, actpress, cord , ncn )
implicit double precision(a-h,o-z)
c arguments are already defined
-----------------------------------------------
dimension vel (maxdf ), press (maxnp), pmat(maxel, 9)
dimension actpress(maxnp), cord (maxnp, ndim)
open(unit=601 , file='cosmocts5', access='sequential',
iform='formatted', status='unknown', iostat=ios
roden=pmat(l,8)
do 6010 imp = 1,nnp
   imp = imp + nnp
   actpress(imp) = roden*press(imp)
write(601,2020) imp , cord(imp,1) , cord (imp,2), 1
   vel(imp),vel(jnp), actpress(imp)
6010 continue
close (601)
3010 format(3i5)
3020 format(i5,2g20.8,2e13.4,e22.8)
return
end subroutine techplot
1 (nnp , vel , press , maxdf , maxnp , icord , 2 pmat , maxel, actpress, cord , ncn , nel , node , ndim )
implicit double precision(a-h.o-z)
c arguments are already defined
-----------------------------------------------
dimension vel (maxdf ), press (maxnp), pmat(maxel, 9)
dimension actpress(maxnp), cord (maxnp, ndim), node(maxel, ncn)
dimension vel (maxnp)
open(unit=601 , file='techplotcts5', access='sequential',
iform='formatted', status='unknown', iostat=ios
compute the magnitude of the resultant velocity
do 1::i,nnp
   j = i
   vm[j] = sqrt((vel(j,1)**2) + (vel(j,2)**2))
end do
write(601,1000)
write(601,2000) nnp, nnel
roden=pmat(l,8)
do 6010 imp = 1,nnp
   imp = imp + nnp
   actpress(imp) = roden*press(imp)
write(601,2020) imp , cord(imp,1) , cord (imp,2), 1
   vel(imp),vel(jnp), actpress(imp)
6010 continue
close (601)
3010 format(3i5)
3020 format(i5,2g20.8,2e13.4,e22.8)
return
end subroutine surfer
1 (nnp, vel, press, maxdf, maxnp, icord, 2 pmat, maxel, actpress, cord, ndim)
implicit double precision(a-h.o-z)
c arguments are already defined
-----------------------------------------------
dimension vel (maxdf ), press (maxnp), pmat(maxel, 9)
dimension actpress(maxnp), cord (maxnp, ndim)
open(unit=602 , file='surferts5', access='sequential',
iform='formatted', status='unknown', iostat=ios
roden=pmat(l,8)
do 6010 imp = 1,nnp
   imp = imp + nnp
   actpress(imp) = roden*press(imp)
write(602,2020) imp , cord(imp,1) , cord (imp,2), 1
   vel(imp),vel(jnp), actpress(imp)
6010 continue
close (602)
3010 format(3i5)
3020 format(i5,2g20.8,2e13.4,e22.8)
return
end subroutine surfer
do i=1,nel
  j=1
  write (603,6000) abs(node(j,1)), abs(node(j,2)), abs(node(j,3))
  write (603,6000) abs(node(j,4)), abs(node(j,5)), abs(node(j,6))
  write (603,6000) abs(node(j,7)), abs(node(j,8)), abs(node(j,9))
  write (603,6000) abs(node(j,10)), abs(node(j,11)), abs(node(j,12))
  end do
  close (603)
1000 format(//'Variables = 'X', 'V', 'D', 'M', 'P';')
2000 format(//'ZONE N=',i5, '//Z=',i5, 'F=FEPOINT, ET=QUADRILATERAL';')
5000 format(e20.12,e20.12,e13.4,e13.4,e13.4,e22.8)
6000 format(4i8)
return
end

其他人也可以根据需要进行注释和完善。
### Deadend Filtration

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A two dimensional finite element model of a non-newtonian isothermal flow using the UVP method.

Deadend Filtration

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   no. of nodes per element = 9
   no. of integration points = 3

*** coordinate system is cartesian (planar) ***

[[[ mesh description data ..........  
   no. of nodal points = 8241
   no. of elements = 2000
   no. of nodal constraints on boundary = 923
   no. of different materials = 1

[[[ uniform body force vector .............  
   grav1 = 0.0000
   grav2 = 0.0000

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node no. max ux node no. min ux
119 0.11209530E-01 87 -0.11209722E-01
node no. max uy node no. min uy
2 0.10000000E+00 5370 -0.79700206E-05
node no. max p node no. min p
4220 0.32875912E+05 5493 -0.15034779E+03

time step 2

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-0.16966476E-01