



PORE-FLOW[®] User's Manual

(version 1.2)

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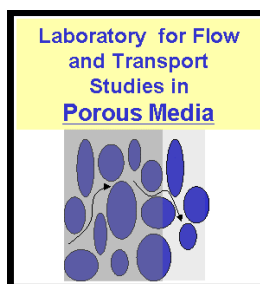


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1. Introduction

PORE-FLOW[®] is a comprehensive computational fluid dynamics tool that solves flow infiltration/wetting problems encountered in industrial porous media. The finite element/control volume method is implemented in the code to simulate flow behind a moving-boundary. The algorithm is efficient and robust for solving the moving-boundary problems in complex domain geometries. The geometry may be 2D or 3D, and the mesh may be structured or unstructured to give maximum flexibility to the user. The porous-medium flow in the code is governed by either Darcy's law or Brinkman equation, depending on the user's choice. PORE-FLOW[®] also can solve the fluid flow problems governed by Stokes or Navier-Stokes equations. The heat flow as well as certain types of reactive flows can also be simulated by the code.

1.1 Features and Benefits

- Easy implementation – Can be used with current software (ANSYS preprocessing and Tecplot post-processing)
- Extensive validation - Modeling tools have been extensively validated using controlled mold filling experiments
- Less modeling error - 30% better agreement compared to current alternatives
- Cheaper - Minimizes cost through optimization of mold design, lower design costs, lower prototyping costs, and lessens need for reworking of molds
- More accurate – Better prediction of pressure and temperature in molds
- Better prediction - Flux-corrected transport for filling simulation removes localized wiggle often seen in solutions and better predictions for permeability
- More versatile - More precise estimation with different mat types such as woven/stitched mats by first solving at the microscale

1. Overview of PORE-FLOW[®] data file

2.1 General remarks

The main purpose of this document is to explain how to create the command file for PORE-FLOW[®]. The command file consists of several command blocks. A template for all of blocks is presented in the corresponding section. The command file has the following properties:

- Lines starting with the symbol “\$” are skipped
- Symbols “_”, “=”, “:”, and “,” are skipped
- Symbol “!” or “\$” can be used to give a comment in a command line
- Only the first EIGHT alphabetic characters of commands are read
- It is not case sensitive
- Blanks are not considered
- The commands written between brackets[] are optional

2.2 Structure of the command file

The command file consists of several groups (blocks) of commands. All of them have a starting word that identifies the group and must finish with the same word following the word END_. There are also several sub-groups of commands that must be provided following the same syntax. The order of the commands within the groups is irrelevant.

The complete list of blocks and sub-blocks of command file is listed as following:

```
$*****
```

```
$ PORE-FLOW: Title
```

```
$*****
```

```
PHYSICAL_PROBLEM  
  NAVIER_STOKES_EQUATIONS  
  BRINKMAN_EQUATIONS  
  DARCY_EQUATION  
  HEAT_EQUATION  
  SPECIES_EQUATION  
  FREE_SURFACE  
END_PHYSICAL_PROBLEM
```

```
PROPERTIES  
  NUM_OF_SETS  
  SET  
  DENSITY
```

VISCOSITY
POROSITY
PERMEABILITY
CONDUCTIVITY
SPECIFIC_HEAT
HEAT_GENERATION
REACTION_RATE
THICKNESS
ENDSET
END_PROPERTIES

MESH_DATA
DIMENSIONS
GEOMETRY
ELEMENTS
COORDINATES
END_MESH_DATA

BOUNDARY_CONDITIONS
INITIAL_CONDITIONS
DIRICHLET_CONDITIONS
NEUMANN_BOUNDARY_CONDITIONS
END_BOUNDARY_CONDITIONS

NUMERICAL_TREATMENT
TIME_DATA
INTEGRATION_POINTS
ITERATION
ERROR
OUT_OF_CORE
NAVIER_STOKES_BRINKMAN
END_NUMERICAL_TREATMENT

OUTPUT
FILE_NAME
FREQUENCY
MUMPS_INFORMATION
END_OUTPUT

3. Physical problem

This block of data can have six sub-blocks depends on the problem needed to be solved. The structure of these blocks and their sub-blocks are:

```
PHYSICAL_PROBLEM
  NAVIER_STOKES_EQUATIONS
  BRINKMAN_EQUATIONS
  DARCY_EQUATION
  HEAT_EQUATION
  SPECIES_EQUATION
  FREE_SURFACE
END_PHYSICAL_PROBLEM
```

3.1 Navier-Stokes equations

All the parameters for NS equations are defined in the following block

```
NAVIER_STOKES_EQUATIONS: ON / OFF, [DOMAIN_NUM=n]
  PRESSURE_ELIMINATION: ON, PENALTY= $\varepsilon$  / OFF
  TRANSIENT: ON / OFF
  CONVECTION: ON / OFF
  STABLIZATION: SUPG / OFF
  BODY_FORCES: ON, GX:  $g_x$ , GY:  $g_y$ , GZ:  $g_z$  / OFF
END_NAVIER_STOKES_EQUATIONS
```

The header of the block '**NAVIER_STOKES_EQUATIONS**' has two options

ON: The NS equations are solved

OFF: The NS equations are not solved

DOMAIN_NUM=*n* is an optional parameter. When NS equations combined with Brinkman equations are solved simultaneously for porous-clear fluid problem, **DOMAIN_NUM=*n*** must be provided. *n* is an integer assigned to the finite elements which lie in the clear-fluid domain.

PRESSURE_ELIMINATION: This command determines if penalty method is used in solution of NS equations or not.

ON: Penalty method¹ is used and **PENALTY= ε** must be provide. ε must be a very small number, e.g. 1e-8.

OFF: Penalty method is not used.

¹ In penalty method, the pressure DOFs do not appear in the final discrete algebraic equations. The continuity equation is incorporated into the momentum equations through a penalty term. Details can be found in FIDAP theory manual.

TRANSIENT: This command determines if the transient effect is considered or not.

ON: Transient term in NS equations is taken into account

OFF: No transient term considered

CONVECTION: This command determines if the inertia term is considered or not.

ON: Inertia term in NS equations is taken into account

OFF: No Inertia term considered. It's in fact Stokes equation

STABLIZATION: This command determines stabilized technique. When the convection is strong, element Reynolds number may be too large to cause solution oscillation. The stabilized technique can stabilize the solution without refining the mesh. When CONVECTION is turned 'ON', it is suggested that the stabilized technique be used.

SUPG: Streamline-Upwinding Petrov Galerkin method

OFF: No stabilized technique is used

BODY_FORCES: the command defines body force

ON: body force is considered. **GX:** x component of \mathbf{g} , **GY:** y component of \mathbf{g} , **GZ:** z component of \mathbf{g} .

OFF: no body force is considered.

3.2 Brinkman equations

All the parameters for Brinkman equations are defined in the following block

```
BRINKMAN_EQUATIONS: ON / OFF, [DOMAIN_NUM= $n$ ]  
  PRESSURE_ELIMINATION: ON, PENALTY= $\varepsilon$  / OFF  
  BODY_FORCES: ON, GX:  $g_x$ , GY:  $g_y$ , GZ:  $g_z$  / OFF  
END_BRINKMAN_EQUATION
```

The header of the block '**BRINKMAN_EQUATIONS**' has two options

ON: The Brinkman equations are solved

OFF: The Brinkman equations are not solved

DOMAIN_NUM= n is an optional parameter. When Brinkman equations combined with NS equations are solved simultaneously for porous-clear fluid problem, **DOMAIN_NUM= n** must be provided. n is an integer assigned to the finite elements which lie in the porous domain.

PRESSURE_ELIMINATION: This command determines if penalty method is used in solution of NS equations or not.

ON: Penalty method is used and **PENALTY**= ε must be provide. ε must be a very small number, e.g. 1e-8.

OFF: Penalty method is not used.

BODY_FORCES: the command defines body force

ON: body force is considered. **GX:** x component of \mathbf{g} , **GY:** y component of \mathbf{g} , **GZ:** z component of \mathbf{g} .

OFF: no body force is considered.

3.3 Darcy equation

The block of commands describing the Darcy equation to be solved is the following:

```
DARCY_EQUATION:ON / OFF
  BODY_FORCES: ON, GX:  $g_x$ , GY:  $g_y$ , GZ:  $g_z$  / OFF
END_DARCY_EQUATION
```

The header of the block '**DARCY_EQUATION**' has two options

ON: The Darcy equation is solved

OFF: The Darcy equation is not solved

BODY_FORCES: the command defines body force

ON: body force is considered. **GX:** x component of \mathbf{g} , **GY:** y component of \mathbf{g} , **GZ:** z component of \mathbf{g} .

OFF: no body force is considered.

3.4 Heat equation

The block of commands describing the heat equation to be solved is the following:

```
HEAT_EQUATION: ON / OFF
  TRANSIENT: ON / OFF
  CONVECTION: ON / OFF
  SHELL_MODEL: ON, WALL_TEMPERATURE= $T_{\text{wall}}$  / OFF
  STABLIZATION: SUPG / FCT / OFF
END_HEAT_EQUATION
```


The header of the block '**HEAT_EQUATION**' has two options

ON: The heat equation is solved

OFF: The heat equation is not solved

TRANSIENT: This command determines if the transient effect is considered or not.

ON: Transient term is taken into account

OFF: No transient term considered

CONVECTION: This command determines if the convective heat transfer is considered or not.

ON: heat convection is taken into account

OFF: No convective term considered. It's in fact pure heat conduction equation

SHELL_MODEL: determines if the thin-wall model used in 3D heat transfer problem.

ON: thin-wall model is considered. In this case, only heat conduction in thickness direction is considered along with heat transfer in-plane. **WALL_TEMPERATURE** represent wall temperature T_{wall} .

OFF: no thin-wall model is used

STABLIZATION: This command determines stabilized techniques. When the heat convection is strong, element Peclet number may be too large to cause solution oscillation (so called convection-dominated convection-diffusion equation). The stabilized techniques can stabilize the solution without refining the mesh. When **CONVECTION** is turned 'ON', it is suggested that the stabilized technique be used.

SUPG: Streamline-Upwinding Petrov Galerkin method

FCT: Flux-Corrected Transport method

OFF: No stabilized technique is used

3.5 Species equation

The block of commands describing the species equation to be solved is the following:

SPECIES_EQUATION: ON / OFF

END_SPECIES_EQUATION

The header of the block '**SPECIES_EQUATION**' has two options

ON: The heat equation is solved

OFF: The heat equation is not solved

3.6 Free surface flow problem

PORE-FLOW[®] uses control volume method to track the flow front. The block of commands describing the free surface-flow problem to be solved is the following:

```
FREE_SURFACE: ON / OFF
  WICKING: ON, CAPILLARY_PRESSURE= $p_a$  / OFF
  DUAL_SCALE: ON / OFF
END_FREE_SURFACE
```

The header of the block '**FREE_SURFACE**' has two options

ON: The free surface is considered

OFF: The free surface is not considered

WICKING: This command determines the wicking flow.

ON: the wicking flow is considered. **CAPILLARY_PRESSURE** must be provided; p_a should be a negative number.

OFF: it's not wicking flow

DUAL_SCALE: The command determines if dual-scale flow is considered

ON: dual-scale flow

OFF: single-scale flow

SINK_MODEL: This command determines the algorithm for solving flow through the dual scale fibrous media. (When **DUAL_SCALE** is turned **ON**, This card must be provided)

MULTISCALE: the algorithm needs two meshes, one is global mesh, and the other one is unit cell mesh.

LUMPED: the algorithm needs only one mesh. The parameters for sink function *must be* defined under '**PHYSICAL PROPERTIES**'.

4. Physical properties

This block of commands provides the physical properties used in simulation.

```
PROPERTIES
  NUM_OF_SETS=n
  SET n
    DENSITY
    VISCOSITY
    POROSITY
    PERMEABILITY
    CONDUCTIVITY
    SPECIFIC_HEAT
    HEAT_GENERATION
    REACTION_RATE
    THICKNESS
    SINK_FUNCTION
  ENDSET n
END_PROPERTIES
```

NUM_OF_SETS: defines the total number of property sets. For example, if there are two different permeabilities in a porous medium, then $n=2$.

SET: determines n^{th} sets of properties

DENSITY: defines the density ρ . If density is a constant, then a float type number ρ is followed by **DENSITY**, e.g. **DENSITY 1000.0**. Density can be defined as a function of variables, for example

DENSITY VARIABLE=TIME, FILLTIME, TEMP, CURE, X, Y, Z

FUN: expression of the function

VISCOSITY: defines the viscosity μ . Similar to Density, viscosity can be defined as either a constant or a function.

POROSITY: defines the porosity ϕ . Similar to Density, porosity can be defined as either a constant or a function.

PERMEABILITY: defines the permeability tensor. If permeability tensor is a constant, **KX**= k_x x-component of permeability tensor, **KY**= k_y y-component of permeability tensor, **KZ**= k_z z-component of permeability tensor, **ROTATION**= θ , rotation angle of principle direction to x, y, z coordinates. If permeability is homogenous, it can be defined as a function similar to density.

CONDUCTIVITY: defines the thermal conductivity tensor. If conductivity tensor is a constant, **CX**= k_x x-component of conductivity tensor, **CY**= k_y y-component of conductivity tensor, **CZ**= k_z z-component of conductivity tensor, **ROTATION**= θ , rotation angle of principle direction to x, y, z coordinates.

SPECIFIC_HEAT: defines the specific heat c_p . Similar to Density, specific heat can be defined as either a constant or a function.

HEAT_GENERATION: defines the heat generation. Similar to Density, heat generation can be defined as either a constant or a function.

REACTION_RATE: defines the reaction rate. Similar to Density, reaction rate can be defined as either a constant or a function.

THICKNESS: defines the thickness of 2D mesh

SINK_FUNCTION: This determines parameters for sink function

$$\frac{dS_{\text{tow}}}{dt} = \frac{A_1 P_{\text{gap}}}{a\mu} \left\{ e^{\left[A_2 (1-S_{\text{tow}})^{A_3} \right]} - 1 \right\}$$

$$\mathbf{A1}=A_1, \mathbf{A2}=A_2, \mathbf{A3}=A_3, \mathbf{B}=a$$

5. Mesh data

This section contains the definition of the computational domain where the problem has to be solved and its discretization.

```
MESH_DATA
  DIMENSIONS
  GEOMETRY
  ELEMENTS
  COORDINATES
END_MESH_DATA
```

5.1 Dimensions

This sub-block contains the following commands

```
DIMENSIONS
  NUMBER_NODES:  ng
  NUMBER_ELEMENTS: ne
  SPACE:  2D /3D
  ELEMENT_TYPE:  TRIA 3 / QUAD 4 / HEXA 8 / TETR 4
  AXISYMMETRY:  YES / NO
END_DIMENSIONS
```

NUMBER_NODES: total number of nodes in FE mesh.

NUMBER_ELEMENTS: total number of elements in FE mesh.

SPACE: defines space dimensions.

ELEMENT_TYPE: defines the element type. ELEMENT_TYPE has the following value depending on the mesh type.

Value	Meaning
TRIA 3	Triangular element with 3 nodes
QUAD 4	Quadrilateral element with 4 nodes
HEXA 8	Hexahedral element with 8 nodes
TETR 4	Tetrahedral element with 4 nodes

AXISYMMETRY: YES-> axi-symmetrical problem, NO. This option is necessary for 2D problems. Note: for axi-symmetrical problem, y direction is always viewed as axis of symmetry.

5.2 Geometry

This block of commands defines the FE mesh.

```

GEOMETRY
  ELEMENTS
    ie, IDdomain, IDset, node1, ..., node n
  END_ELEMENTS
  COORDINATES
    in, LOCX, LOCY, LOCZ
  END_COORDINATES
END_GEOMETRY

```

ELEMENTS: defines the connectivity of each element.

ie: element number

IDdomain: domain number corresponding to DOMAIN_NUM=*n* in Section 3.1 and 3.2

IDset: property set number corresponding to SET *n* in Section 4

node1, ..., node *n*: list of nodes belonging to element *ie*

COORDINATES: defines the coordinates of nodes.

in: node number

LOCX: *x*-coordinate of node *in*

LOCY: *y*-coordinate of node *in*

LOCZ: *z*-coordinate of node *in*

NOTE: To make the command file compact and neat, the sub-blocks of ELEMENTS and COORDINATES can be included in another file. The path and file name need to be provided in GEOMETRY, e.g.,

```

GEOMETRY
  INCLUDE C:\*****\***\XXX.XX
END_GEOMETRY

```

6. Boundary conditions

This block contains the definition of the boundary conditions for the problem to be solved.

```
BOUNDARY_CONDITIONS
  INITIAL_CONDITIONS
  DIRICHLET_CONDITIONS
  NEUMANN_CONDITIONS
  FREE_SURFACE_CONDITIONS
END_BOUNDARY_CONDITIONS
```

6.1 Initial conditions

The block defines the initial conditions for transient analysis.

```
INITIAL_CONDITIONS
  VX= $V_x$ , VY= $V_y$ , VZ= $V_z$ , TEMPERATURE= $T_0$ , CURE= $\alpha_0$ 
END_INITIAL_CONDITIONS
```

VX: initial velocity in x -direction V_x

VY: initial velocity in y -direction V_y

VZ: initial velocity in z -direction V_z . For 2D problems, do not include this term.

TEMPERATURE: initial temperature. If HEAT_EQUATION is turned 'OFF', do not include this term.

CURE: initial degree of cure. If SPECIES_EQUATION is turned 'OFF', do not include this term.

NOTE: for pure heat transfer problems, the INITIAL_CONDITIONS can be used to give the velocity field.

6.2 Dirichlet condition

The block defines the Dirichlet boundary conditions. Note: for NS equations, Brinkman equations, Dirichlet condition specifies the velocity on the boundary, while for Darcy equation, Dirichlet condition specifies the pressure value on the boundary.

```
DIRICHLET_CONDITIONS
  in, IDvx, IDvy, IDvz, IDT, IDcure,  $V_x$ ,  $V_y$ ,  $V_z$ ,  $T$ ,  $\alpha$  (NS or Brinkman)
  in, IDP, IDT, IDcure,  $P_a$ ,  $T$ ,  $\alpha$  (Darcy equation)
END_DIRICHLET_CONDITIONS
```

in: node number.

IDvx: code for boundary condition of x -velocity. IDvx is either 0 or 1. 0 means x -velocity is free. 1 means the x -velocity is prescribed.

IDvy: code for boundary condition of y -velocity. The possibilities of IDvy are same as IDvx.

IDvz: code for boundary condition of z -velocity. The possibilities of IDvz are same as IDvx. For 2D problem, do not include this term.

IDP: code for boundary condition of pressure for Darcy equation. The possibilities of IDP are same as IDvx.

IDT: code for boundary condition of temperature. The possibilities of IDT are same as IDvx. If HEAT_EQUATION is turned '**OFF**', do not include this term.

IDcure: code for boundary condition of cure. The possibilities of IDcure are same as IDvx. If SPECIES_EQUATION is turned '**OFF**', do not include this term.

V_x : x -velocity of node in .

V_y : y -velocity of node in .

V_z : z -velocity of node in . For 2D problem, do not include this term.

P_a : pressure of node in .

T : temperature of node in . If HEAT_EQUATION is turned '**OFF**', do not include this term.

α : degree of cure of node in . If SPECIES_EQUATION is turned '**OFF**', do not include this term.

6.3 Neumann conditions

The block defines the Neumann boundary conditions. Note: for NS equations, Brinkman equations, Neumann condition specifies the pressure on the boundary, while for Darcy equation, Neumann condition specifies flow rate on the boundary.

```
NEUMANN_CONDITIONS
  in, IDP, IDFlux,  $P_a$ , Flux (for NS or Brinkman)
  in, IDF, IDFlux,  $Q$ , Flux (for Darcy equation)
END_NEUMANN_CONDITIONS
```

in: node number.

IDP: code for boundary condition of pressure. IDP is either 0 or 1. 0 means pressure is free. 1 means that pressure is prescribed.

IDF: code for boundary condition of flow rate. IDF is either 0 or 1. 0 means pressure is free. 1 means that flow rate is prescribed.

P_a : pressure applied on node *in*.

Q : flow rate applied on node *in*.

Flux: heat flow applied on node *in*. If HEAT_EQUATION is turned '**OFF**', do not include this term.

6.4 Free Surface Conditions

This block defines the inlet and outlet boundaries. The block is necessary only when FREE_SURFACE is turned "**ON**".

```
FREE_SURFACE_CONDITIONS
  in, ID
END_FREE_SURFACE_CONDITIONS
```

in: node number.

ID: code for inlet or outlet. ID is either 0 or 1. 0 means node *in* belongs to inlet. 1 means node *in* belongs to outlet.

NOTE: To make the command file compact and neat, the sub-blocks of DIRICHLET_CONDITIONS, NEUMANN_CONDITIONS, and FREE_SURFACE_CONDITIONS can be included in a file. The path and file name need to be provided in BOUNDARY_CONDITIONS, e.g.

```
BOUNDARY_CONDITIONS
  INITIAL_CONDITIONS
    VX=0, VY=0, VZ=0
  END_INITIAL_CONDITIONS
  INCLUDE C:\*****\***\XXX.XX
END_BOUNDARY_CONDITIONS
```

7. Numerical Treatment

The block determines the parameters in numerical solution.

```
NUMERICAL_TREATMENT
  TIME_DATA
  INTEGRATION_POINTS
  ITERATION
  ERROR
  OUT_OF_CORE
  NAVIER_STOKES_BRINKMAN
    BUBBLE_FORMULATION
    PRESSURE_INTERPOLATION
  END_NAVIER_STOKES
END_NUMERICAL_TREATMENT
```

TIME_DATA: determines the time integration algorithm for transient analysis, which has following keywords:

INITIAL_TIME: initial time

FINAL_TIME: end of time

TIME_STEP_SIZE: time increment in each step

THETA: an adjustable parameter varying between 0 and 1. THETA can be 0 (forward), 0.5 (Crank-Nicolson), 1 (backward).

Note: all the keywords including TIME_DATA should be in the same line, for example,

TIME_DATA: INITIAL_TIME=0.0, FINAL_TIME=100, TIME_STEP_SIZE=1.e-1, THETA=0.5

INTEGRATION_POINTS: the number of integral points for each element. It is an integer number which is determined by the element type of Section 5.1.

Element type	# Integration points
TRIA 3	4
QUAD 4	4 or 9
HEXA 8	8 or 27
TETR 4	1, 4, 5, 10, or 11

ITERATION: iteration method. It can be following value

PICARD: fixed point iteration method

NEWTON: Newton iteration method

PICNEW n : the combination of Picard and Newton method. Here n means the number of iteration using Picard method. In this method, the first n steps use Picard method followed by Newton method. When PICNEW is used, n must be provided.

ERROR: criterion for iteration method. When the difference between the solutions of successive iterations is less than the number, the convergence is reached. For example

$$\frac{\|\mathbf{u}_{i+1} - \mathbf{u}_i\|}{\mathbf{u}_i} \leq \varepsilon$$

where \mathbf{u} is solution, subscript i is iteration number, ε is error of iteration.

OUT_OF_CORE: ‘ON’ or ‘OFF’. When the problem is very large, the in-core memory requirement may exceed the capacity of the computer. Turning on OUT_OF_CORE can use hard drive to store the matrix.

7.1 Numerical treatment for NS and Brinkman equations

This block determines the parameters just for NS and Brinkman equation. If NAVIER_STOKES_EQUATIONS or BRINKMAN_EQUATIONS is turned ‘ON’, the block must be included. Otherwise, it is not necessary to include the whole block.

```
NAVIER_STOKES_BRINKMAN
  BUBBLE_FORMULATION: ON / OFF
  PRESSURE_INTERPOLATION: n
END_NAVIER_STOKES
```

BUBBLE_FORMULATION: when tetrahedral elements with 4 nodes are used to solve NS and Brinkman equation, BUBBLE_FORMULATION should be turned ‘ON’. For other types of elements, it should be turn ‘OFF’.

PRESSURE_INTERPOLATION: This defines the interpolation used for the pressure. An integer must be provided. Now it can be only 1.

8. Output

PORE-FLOW[©] uses TECPLOT as post processor.

OUTPUT

FILE_NAME

FREQUENCY: STEP= n

MUMPS_INFORMATION: ON /OFF

END_OUTPUT

FILE_NAME: file name for output file.

FREQUENCY: for transient analysis or filling analysis, this parameter determines how often the solution is written into the solution file.

MUMPS_INFORMATION: PORE-FLOW[©] uses MUMPS to solve the algebraic equation. When MUMPS_INFORMATION is turn 'ON', the solution information coming from MUMPS will be printed on the screen. Otherwise, no solution information is printed.

9. Preprocessing

In order to run this software, one needs three following files:

1. Command file
2. Mesh file
3. Boundary condition file

The command file was discussed in the previous sections. We discuss how to make the mesh and boundary condition files in this section:

9.1 Mesh file

Mesh file has two parts; the first part is in the following format:

```
ELEMENTS
element number, Domain ID, Property ID, local node 1, ....., local node 8
END_ELEMENTS
```

The first three columns are the element #, domain ID and property ID. The next columns are nodes associated with the element in the first column. Therefore, we have 4 nodes for 2D and 8 nodes for 3D simulation. The second part of mesh file is coordinate, which gives the coordinate information for nodes. Here is the format:

```
COORDINATES
node number, x coordinate, y coordinate, z coordinate
END_COORDINATES
```

In case of working in 2D, then one of these columns is zero or there are just two columns. In case, there is one column, the other column is considered to be zero. If the mesh was made in ANSYS, then above data can be achieved through following command:

Preprocessor>>Archive Model>>Write>>Data to Archive>>pick GEOM; then in “Archive file” give a name for output file.

We may need to delete some rows or columns from GEOM file. For this purpose, UltraEdit is a powerful editing software. Following is a sample 2D mesh file:

ELEMENTS

\$ element number, Domain ID, Property ID, local node 1,, local node 4

```
1 1 1 1 3 81 80
2 1 1 3 4 100 81
3 1 1 4 5 119 100
4 1 1 5 6 138 119
5 1 1 6 7 157 138
6 1 1 7 8 176 157
7 1 1 8 9 195 176
8 1 1 9 10 214 195
9 1 1 10 11 233 214
10 1 1 11 12 252 233
```

.
.
.

```
393 1 1 308 327 49 50
394 1 1 327 346 48 49
395 1 1 346 365 47 48
396 1 1 365 384 46 47
397 1 1 384 403 45 46
398 1 1 403 422 44 45
399 1 1 422 441 43 44
400 1 1 441 41 22 43
```

END_ELEMENTS

COORDINATES

\$ node number, x coordinate, y coordinate, z coordinate

```
1 0.00000000
2 0.177800000
3 8.890000000E-03
4 1.778000000E-02
5 2.667000000E-02
6 3.556000000E-02
7 4.445000000E-02
8 5.334000000E-02
9 6.223000000E-02
10 7.112000000E-02
```

.
.
.

```
435 0.168910000 0.115570000
436 0.168910000 0.124460000
```

```

437 0.168910000 0.133350000
438 0.168910000 0.142240000
439 0.168910000 0.151130000
440 0.168910000 0.160020000
441 0.168910000 0.168910000
END_COORDINATES

```

9.2 Boundary condition file

Boundary condition has two or three of following parts:

```

DIRICHLET_CONDITIONS
  in, IDvx, IDvy, IDvz, IDT, IDcure, Vx, Vy, Vz, T,  $\alpha$  (NS or Brinkman)
  in, IDP, IDT, IDcure, Pa, T,  $\alpha$  (Darcy equation)
END_DIRICHLET_CONDITIONS

```

Or

```

NUMANN_CONDITIONS
  in, IDP, IDFlux, Pa, Flux (for NS or Brinkman)
  in, IDF, IDFlux, Q, Flux (for Darcy equation)
END_NEUMANN

```

Or

```

FREE_SURFACE_CONDITIONS
  in, ID
END_FREE_SURFACE_CONDITIONS

```

The details of above characters are explained in sections 6.2, 6.3, and 6.4. If the mesh was made in ANSYS, then above described node numbers can be obtained through following command:

- 1) Selecting the boundary of the object. In a 2D mesh, one can use following commands to select a boundary line:


```
Select>>Entities>>Lines>>By Num/Pick>>click on boundary line(s)>>OK
```
- 2) Select the nodes connected to previous selected boundary:


```
Select>>Entities>>Nodes>>Attached to>>Lines, all>>OK
```
- 3) Output the node information:


```
List>>Nodes>>OK
```

Following is a sample boundary condition file for mold filling simulation under constant pressure injection:

```
DIRICHLET_CONDITIONS
 1 1 20000
42 1 20000
62 1 20000
63 1 20000
.
.
.
77 1 20000
78 1 20000
79 1 20000
80 1 20000
END_DIRICHLET_CONDITIONS

FREE_SURFACE_CONDITIONS
 1 0
42 0
62 0
63 0
.
.
.
37 1
38 1
39 1
40 1
41 1
END_FREE_SURFACE_CONDITIONS
```


10. Numerical examples

10.1 Wicking Flow through swelling medium

The problem is a wicking flow through a swelling medium involving a moving boundary. The gravity effect is taken into consideration. The permeability is changing with time as follows

$$P_c = -96271.21679 \text{ Pa (capillary pressure)}$$

$$K/\varepsilon_0 * 1E14 = 0.04508552357 t - 1.673195381 t^{1/2} + 23.62425661 \text{ m}^2$$

The viscosity and density of the liquid are $\mu=0.000911 \text{ Pa}\cdot\text{s}$ and 1000 kg/m^3 . Porosity ε_0 is 0.5. In this case, 2D analysis is carried out. Quadrilateral elements are used to discretize the computational domain. Total numbers of nodes and elements are 1111 and 1000, respectively. The mesh model is shown in figure 1.

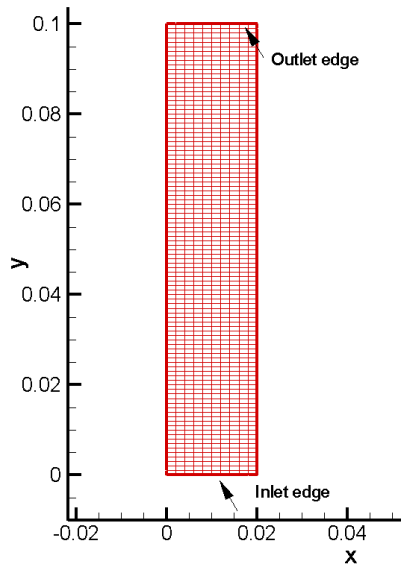


Figure 1 : FE mesh model.

The command file is listed here

```

$*****
PORE-FLOW 2D swelling media flow problem
$*****
PHYSICAL_PROBLEM
$-----
DARCY_EQUATION: ON
  BODY_FORCES: ON,GX:0., GY:-9.8, GZ:0. ← Consider gravity
END_DARCY
$-----
FREE_SURFACE: ON ← FREE_SURFACE must be turned on, since it's a moving boundary problem
  WICKING: ON, CAPILLARY_PRESSURE= -96271.21679
  DUAL_SCALE:OFF ← Wicking flow and capillary pressure
END_FREE_SURFACE
$-----

```

```

END_PHYSICAL_PROBLEM
$*****
PROPERTIES
NUM_OF_SETS=1 → Since the material is homogenous, Only one set of property
is used in the simulation.
$-----
SET 1
  DENSITY: 1000
  VISCOSITY: .000911
  POROSITY: .5
  PERMEABILITY: VARIABLE=FILLTIME → Permeability is function
of filling time.
  FUN: (0.04508552357*FILLTIME-1.673195381*FILLTIME^(.5)+23.62425661)*1e-14*0.5
  THICKNESS: 1. ! valid for 2D filling analysis → Function expression
ENDSET 1
END_PROPERTIES → '! ' can be used to give comment in a command line
$*****
MESH_DATA
$-----
DIMENSIONS
  NUMBER_NODES: 1111
  NUMBER_ELEMENTS: 1000
  SPACE: 2D
  ELEMENT_TYPE: QUAD 4
  AXISYMMETRY: NO
END_DIMENSIONS
$-----
GEOMETRY
  INCLUDE C:\hua tan\code validation\example\swell.qu → Mesh data is included in swell.qu.
  END_GEOMETRY → When running the example, note
the path of swell.qu.
$-----
END_MESH_DATA
$*****
BOUNDARY_CONDITIONS
$-----
  INITIAL_CONDITIONS → INITIAL_CONDITIONS does not work in this case.
    VX=0. VY=0. VZ=0.
  END_INITIAL
  INCLUDE C:\hua tan\code validation\example\swell.ini → B.C. data is included in swell.ini.
  → When running the example, note
the path of swell.ini.
$-----
END_BOUNDARY_CONDITIONS
$*****
NUMERICAL_TREATMENT
  TIME_DATA: INITIAL_TIME=0.0 FINAL_TIME=5 TIME_STEP_SIZE=1. THETA=0.5
  INTEGRATION_POINTS: 4
  ITERATION: PICARD → TIME_DATA, ITERATION, and
ERROR → ERROR are not necessary in this case.
  ERROR: 5.D-5
  OUT_OF_CORE: OFF
END_NUMERICAL_TREATMENT
$*****
OUTPUT
  FILE_NAME: global.out
  FREQUENCY: STEP=5 → The solution is output every 5 steps
  MUMPS_INFORMATION:Off
END_OUTPUT
$*****

```

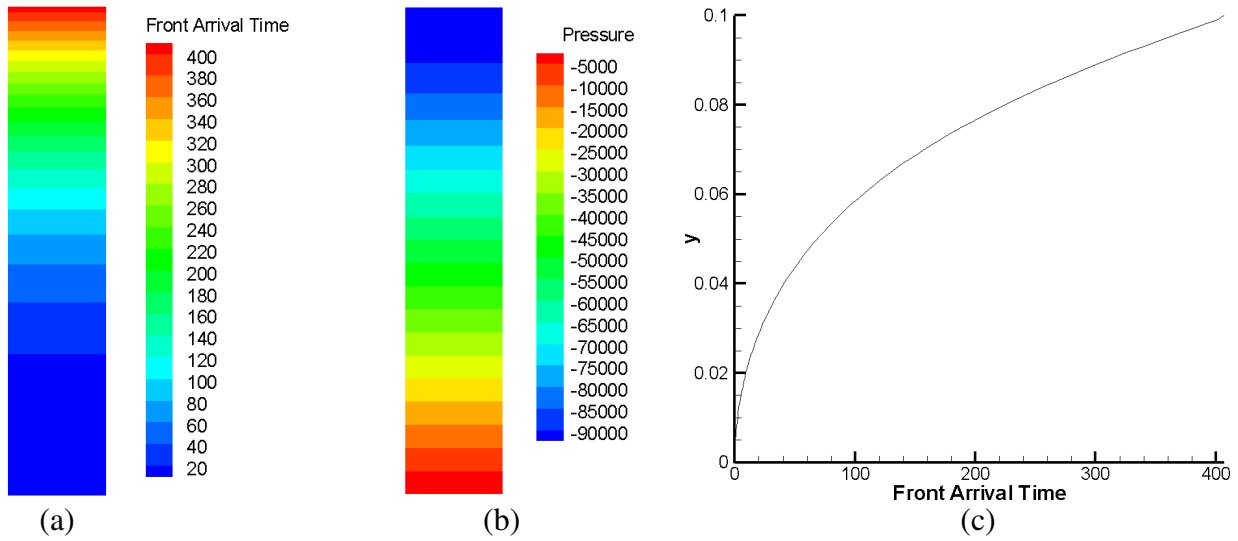


Figure 2. (a) the flow-front evolution, (b) the pressure distribution at the end of filling, (c) flow-front position vs time

10.2 Permeability prediction

A unit cell model of bi-axial fabrics is constructed to predict the permeability. The problem is steady-state. The longitudinal permeability K_{\parallel} and transverse permeability K_{\perp} of fiber tow are assumed to be $5e-10 \text{ m}^2$ and $1e-10 \text{ m}^2$, respectively. The liquid viscosity is 1 Pa s . The flow in inter-tow gap region is modeled using Stokes equations, while the flow in the intra-tow region is modeled using Brinkman equation. Therefore, there are two different computational domain (one for Stokes equation, the other one for Brinkman equation), and three sets of properties (one for gap region, one for tow parallel to z-direction, one for tow parallel to x-direction). The FE model of the unit cell is shown in Figure 3. It has 17572 nodes and 15320 hexahedral elements. The pressure boundary conditions of 100 Pa and 0 Pa are applied on the opposite surfaces of the unit cell along the flow direction to simulate the z-direction flow. Symmetric boundary conditions are imposed on the remaining surfaces of the unit cell.

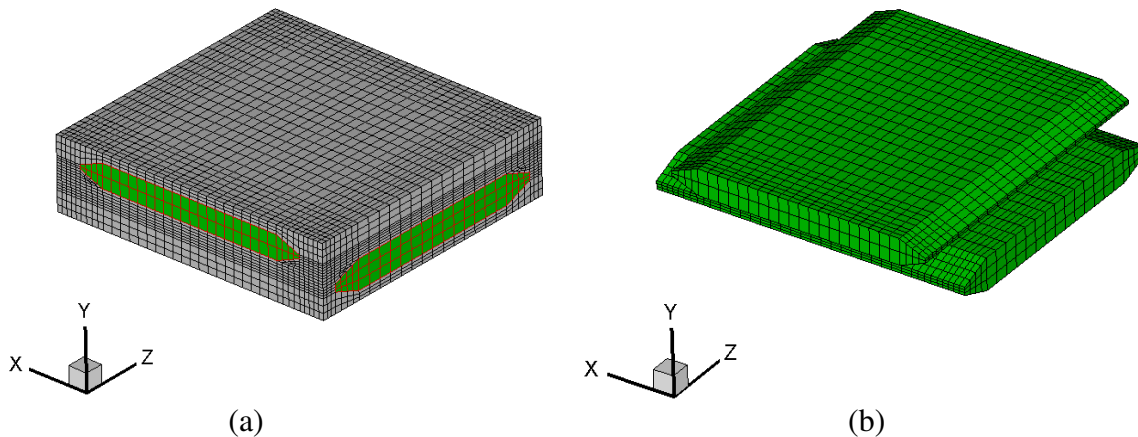


Figure 3 : (a) FE mesh of unit-cell, (b) FE mesh of fiber tow region.

The command file is listed as

```

$*****
PORE-FLOW: PERMEABILITY PREDICTION PROBLEM
$*****
PHYSICAL_PROBLEM
$-----
NAVIER_STOKES_EQUATIONS: ON, DOMAIN_NUM=1 → Domain 1 is Stokes equation
PRESSURE_ELIMINATION: ON PENALTY=1D-8
TRANSIENT: OFF
CONVECTION: OFF ← Convection is turned off, so the inertial term is not considered.
STABILIZATION: OFF ← Convection is turned off, hence there is no need to stabilize
BODY_FORCES: OFF oscillatory solution caused by the convection term.
END_NAVIER_STOKES_EQUATIONS

```



```

OUT_OF_CORE: OFF
$-----
NAVIER_STOKES_BRINKMAN
  BUBBLE_FORMULATION: OFF $/ON
  PRESSURE_INTERPOLATION: 1
END_NAVIER_STOKES
$-----
END_NUMERICAL_TREATMENT
$*****
OUTPUT
  FILE_NAME: global.out
  FREQUENCY: STEP=8
  MUMPS_INFORMATION: OFF
END_OUTPUT
$*****

```

← Since it is a steady-state problem, FREQUENCY does not work in this case.

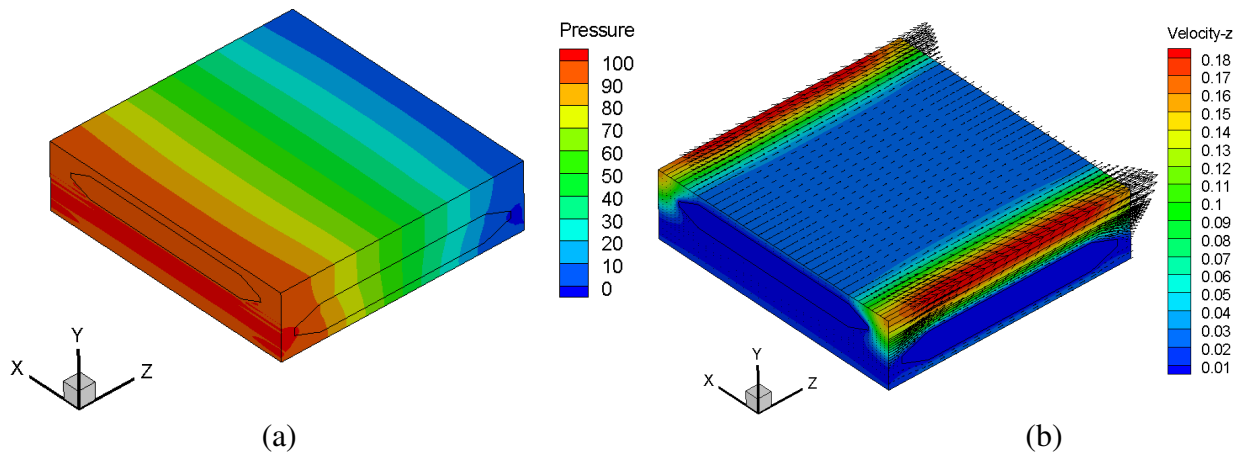


Figure 4 : (a) pressure distribution across the unit-cell, (b) z-velocity and velocity vector.

10.3 Flow in an elbow pipe

The flow through an elbow pipe is analyzed in this study. The problem is three dimensional Navier-Stokes flow. The liquid density and viscosity are 1000 kg/m^3 and 0.3 Pa s , respectively. The FE model is shown in figure 5. There are 2223 nodes and 1824 hexahedral elements in the model. The pressure boundary conditions of 1000 Pa and 0 Pa are applied on the inlet and outlet surfaces, respectively. The other surfaces are non-slip boundary condition.

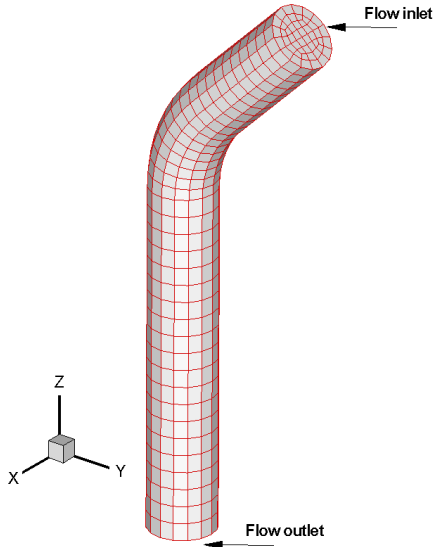


Figure 5: FE mesh of elbow pipe.

The command file is listed as

```

$*****
PORE-FLOW: ELBOW 3D PROBLEM
$*****
PHYSICAL_PROBLEM
$-----
  NAVIER_STOKES_EQUATIONS: ON
    PRESSURE_ELIMINATION: on PENALTY=1D-8
    TRANSIENT: OFF
    CONVECTION: ON
    STABLIZATION: SUPG ← SUPG is used to stabilize the numerical solution
    BODY_FORCES: OFF,
  END_NAVIER_STOKES_EQUATIONS
$-----
END_PHYSICAL_PROBLEM
$*****
PROPERTIES
  NUM_OF_SETS=1
$-----
  SET 1
    DENSITY:1000
    VISCOSITY: .3

```

```

ENDSET 1
$-----
END_PROPERTIES
$*****
MESH_DATA
$-----
DIMENSIONS
  NUMBER_NODES: 2223
  NUMBER_ELEMENTS: 1824
  SPACE: 3D
  ELEMENT_TYPE: HEXA 8
  AXISYMMETRY: NO
END_DIMENSIONS
$-----
GEOMETRY
  INCLUDE C:\hua tan\incompressiveflow\ELBOW.INI
END_GEOMETRY
$-----
END_MESH_DATA
$*****
BOUNDARY_CONDITIONS
$-----
INITIAL_CONDITIONS
  VX=0 VY=0 VZ=0
END_INITIAL
  INCLUDE C:\hua tan\incompressiveflow\ELBOW.INI
$-----
END_BOUNDARY_CONDITIONS
$*****
NUMERICAL_TREATMENT
  TIME_DATA: INITIAL_TIME=0.0 FINAL_TIME=100. TIME_STEP_SIZE=1.d-1 THETA=0.5
  INTEGRATION_POINTS: 8
  ITERATION: PICNEW
  ERROR: 5.D-5
$-----
NAVIER_STOKES_BRINKMAN
  BUBBLE_FORMULATION: OFF
  PRESSURE_INTERPOLATION: 1
END_NAVIER_STOKES
$-----
END_NUMERICAL_TREATMENT
$*****
OUTPUT
  FILE_NAME: global.out
  FREQUENCY: STEP=8
END_OUTPUT
$*****

```

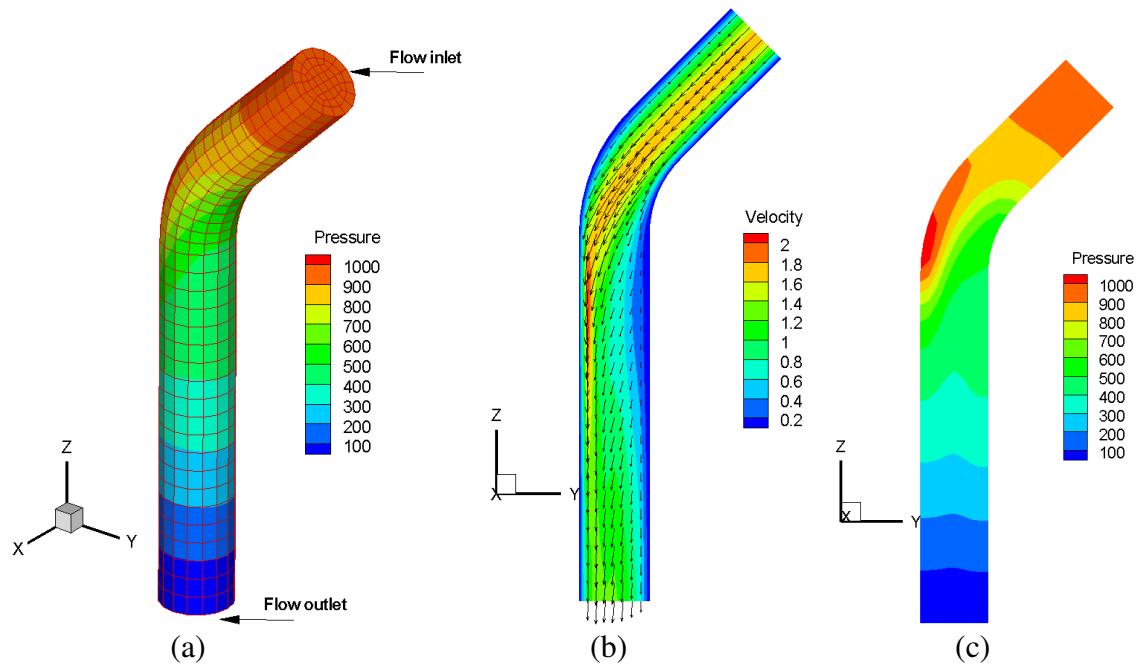



Figure 6 : (a) pressure distribution of the elbow, (b) velocity distribution and vector on the middle-plane of the elbow, (c) pressure distribution on the middle-plane.

10.4 Heat flow between two parallel plates

The problem is a cold liquid of 20°C flowing between two infinitely large plates with a higher constant temperature of 75°C . The liquid density, viscosity, conductivity and specific heat are 10 kg/m^3 , 1 Pa s , $1\text{ W/m }^{\circ}\text{K}$, and $1000\text{ J/kg }^{\circ}\text{K}$, respectively. The inlet flow velocity is 1 m/s . Since the domain is symmetrical, only half of the domain is discretized using FE mesh as shown in figure 7. For this problem, the NS equations are first solved to obtain the velocity field, then the heat transfer equation is solved to obtain the temperature field.

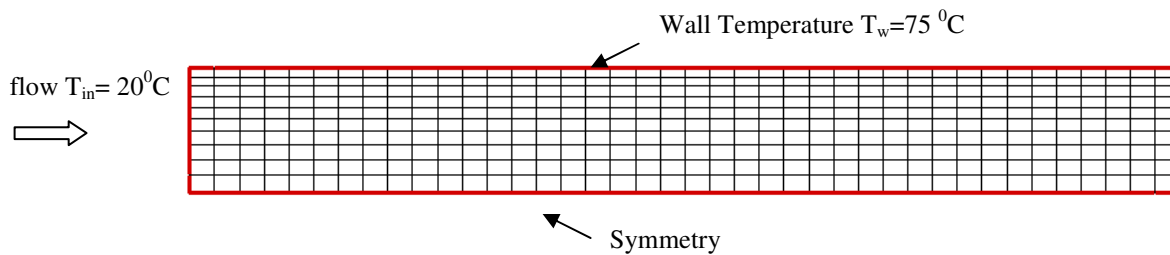


Figure 7: FE mesh

The command file is listed as

```

$*****
$PORE-FLOW 2D heat transfer problem
$*****
PHYSICAL_PROBLEM
$-----
  NAVIER_STOKES_EQUATIONS: ON
    PRESSURE_ELIMINATION: ON, PENALTY=1D-8
    TRANSIENT: OFF
    CONVECTION: ON
    STABLIZATION: SUPG
    BODY_FORCES: OFF
  END_NAVIER_STOKES_EQUATIONS
$-----
  HEAT_EQUATION: ON
    TRANSIENT: OFF
    CONVECTION: ON
    SHELL_MODEL: OFF
    STABLIZATION: SUPG
  END_HEAT_EQUATION
$-----
END_PHYSICAL_PROBLEM
$*****
PROPERTIES
NUM_OF_SETS=1
$-----
SET 1
  DENSITY: 10

```

} Defines the NS equation

} Defines the heat transfer equation

```

VISCOSITY: 1.
CONDUCTIVITY: CX=1, CY=1, CZ=1,ROTATION=0
SPECIFIC_HEAT:1000
HEAT_GENERATION: 0.
THICKNESS: 1d-2
ENDSET 1
END_PROPERTIES
$*****
MESH_DATA
$-----
  DIMENSIONS
    NUMBER_NODES: 451
    NUMBER_ELEMENTS: 400
    SPACE: 2D
    ELEMENT_TYPE: QUAD 4
    AXISYMMETRY: NO
  END_DIMENSIONS
$-----
  GEOMETRY
    INCLUDE C:\hua tan\code validation\example\plateflow2D.qu
  END_GEOMETRY
$-----
END_MESH_DATA
$*****
BOUNDARY_CONDITIONS
$-----
  INITIAL_CONDITIONS
    VX=0. VY=0. VZ=0. TEMPERATURE=293
  END_INITIAL
  INCLUDE C:\hua tan\code validation\example\plateflow2D.ini
$-----
END_BOUNDARY_CONDITIONS
$*****
NUMERICAL_TREATMENT
  TIME_DATA: INITIAL_TIME=0.0 FINAL_TIME=100. TIME_STEP_SIZE=1D-2 THETA=0.5
  INTEGRATION_POINTS: 4
  ITERATION: NEWTON
  ERROR: 6.D-5
  OUT_OF_CORE: OFF
$-----
  NAVIER_STOKES_BRINKMAN
    BUBBLE_FORMULATION: OFF
    PRESSURE_INTERPOLATION: 1
  END_NAVIER_STOKES
$-----
END_NUMERICAL_TREATMENT
$*****
OUTPUT
  FILE_NAME: global.out
  FREQUENCY: STEP=5
  MUMPS_INFORMATION: OFF
END_OUTPUT
$*****

```

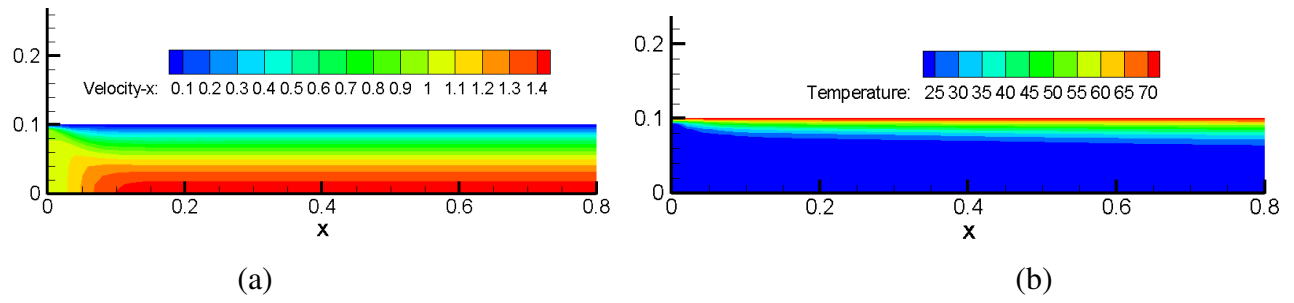


Figure 8: (a) velocity distribution, (b) temperature distribution.

10.5 Mold filling simulation

The problem is a mold of 7"×7" (0.1778×0.1778m) mold that is filling with a resin or a test liquid. The porosity is 0.5 and the density and viscosity of liquid are 860 kg/m³ and 0.244 Pa.s, respectively. The permeability of fibermats is 1e-7 m² and the injection pressure is 20 kPa. We want to study the flow of resin in such a simple 2-d mold. The domain is discretized using FE mesh as shown in Figure 9. For this problem, the Darcy equation and continuity equations are solved to find the pressure distribution. Then the liquid front location and velocity will be found using Darcy's law.

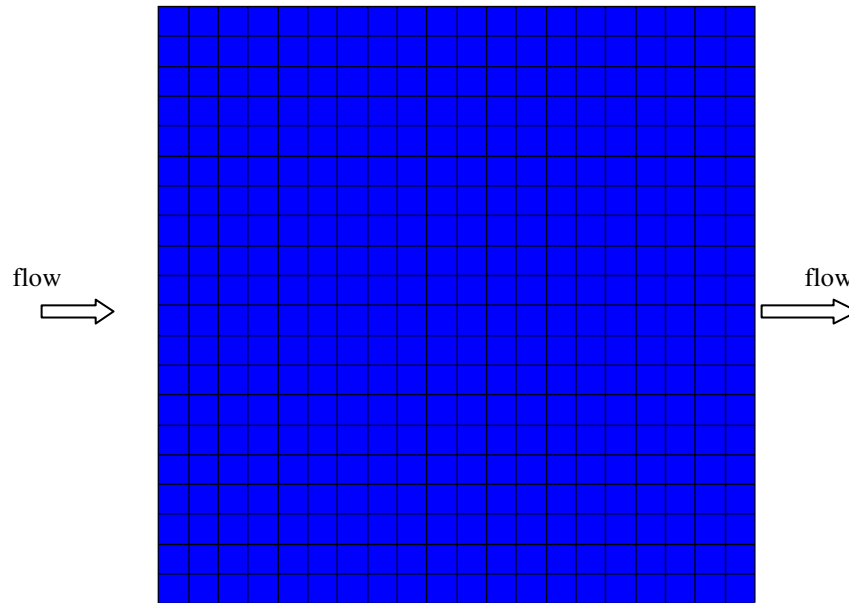


Figure 9: FE mesh

The command file is listed as

```
$*****  
PORE-FLOW 2D mold filling flow problem  
$*****  
PHYSICAL_PROBLEM  
$-----  
DARCY_EQUATION: ON  
  BODY_FORCES: ON, GX:0., GY:0., GZ:0.  
END_DARCY  
$-----  
FREE_SURFACE: ON  
  WICKING: OFF  
  DUAL_SCALE: OFF  
END_FREE_SURFACE  
$-----  
END_PHYSICAL_PROBLEM
```

```

$*****
PROPERTIES
NUM_OF_SETS=1
$-----
SET 1
  DENSITY: 860
  VISCOSITY: .244
  POROSITY: .5
  PERMEABILITY: KX=1e-7, KY=1e-7, KZ=1e-7, ROTATION=0
  THICKNESS: 1. ! valid for 2D filling analysis
ENDSET 1
END_PROPERTIES
$*****
MESH_DATA
$-----
  DIMENSIONS
    NUMBER_NODES: 441
    NUMBER_ELEMENTS: 400
    SPACE: 2D
    ELEMENT_TYPE: QUAD 4
    AXISYMMETRY: NO
  END_DIMENSIONS
$-----
  GEOMETRY
    INCLUDE C:\POREFLOW\example\Mold_Geom_2D.dat
  END_GEOMETRY
$-----
END_MESH_DATA
$*****
BOUNDARY_CONDITIONS
$-----
  INITIAL_CONDITIONS
    VX=0. VY=0. VZ=0.
  END_INITIAL
  INCLUDE C:\POREFLOW\example\Mold_BC_2D.dat
$-----
END_BOUNDARY_CONDITIONS
$*****
NUMERICAL_TREATMENT
  TIME_DATA: INITIAL_TIME=0.0 FINAL_TIME=5 TIME_STEP_SIZE=1. THETA=0.5
  INTEGRATION_POINTS: 4
  ITERATION: PICARD
  ERROR: 5.D-5
  OUT_OF_CORE: OFF
END_NUMERICAL_TREATMENT
$*****
OUTPUT
  FILE_NAME: Mold2D_RESULT.dat
  FREQUENCY: STEP=5
  MUMPS_INFORMATION:Off
END_OUTPUT
$*****

```

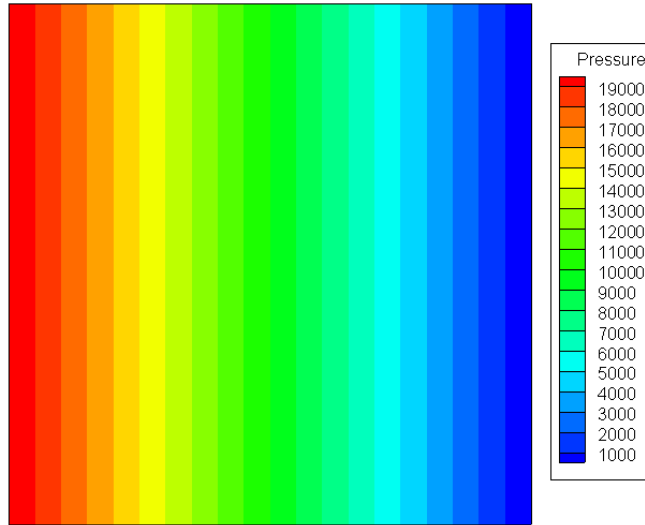


Figure 10: Pressure distribution

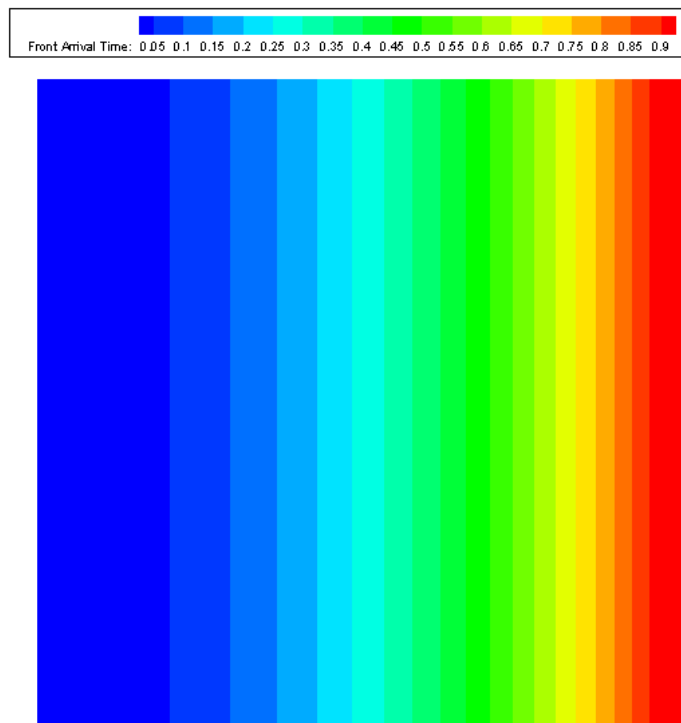


Figure 11: Liquid front location versus time

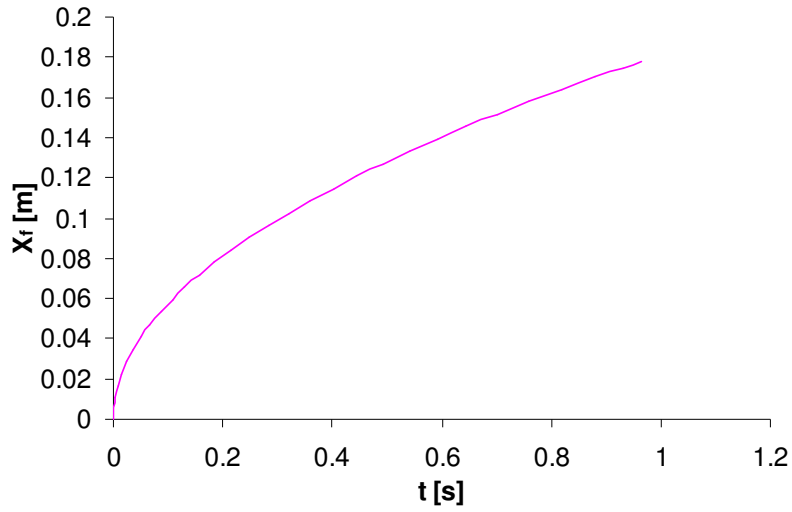


Figure 12: Liquid-front location versus time

More simulation results for mold filling

Geometry, Grid and Boundary Conditions: Initial pressure P=20000

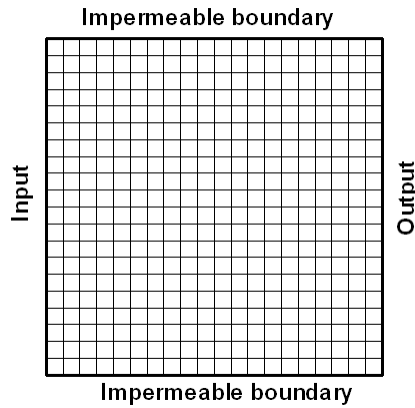


Fig 13 Boundary and Grid

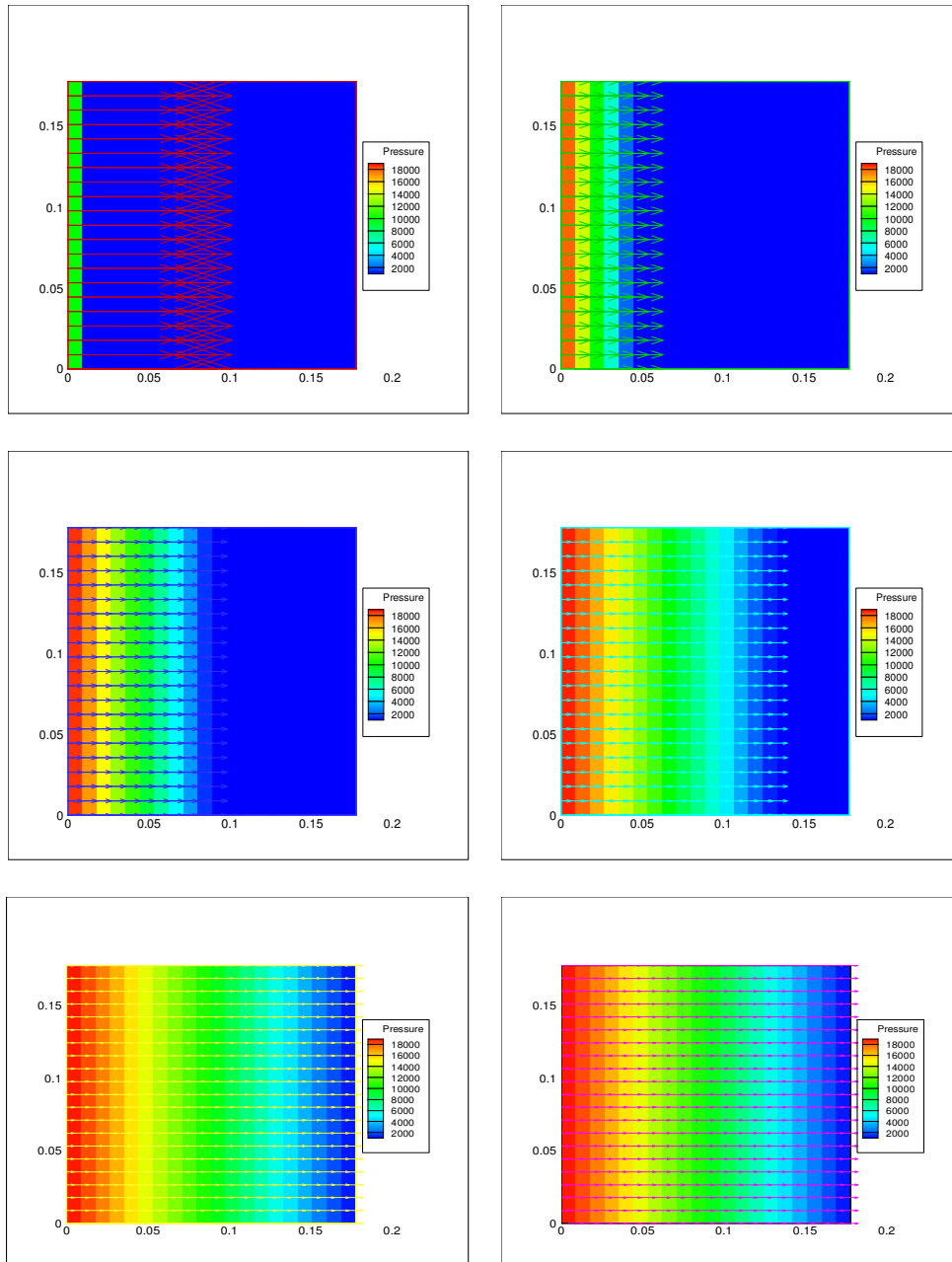


Fig 14 Distribution of Velocity and Pressure in a porous media

Rectangular Geometry Results:

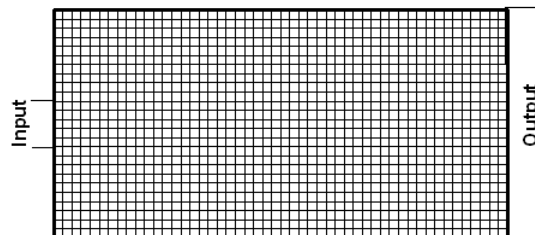


Fig 15 Boundary and Grid

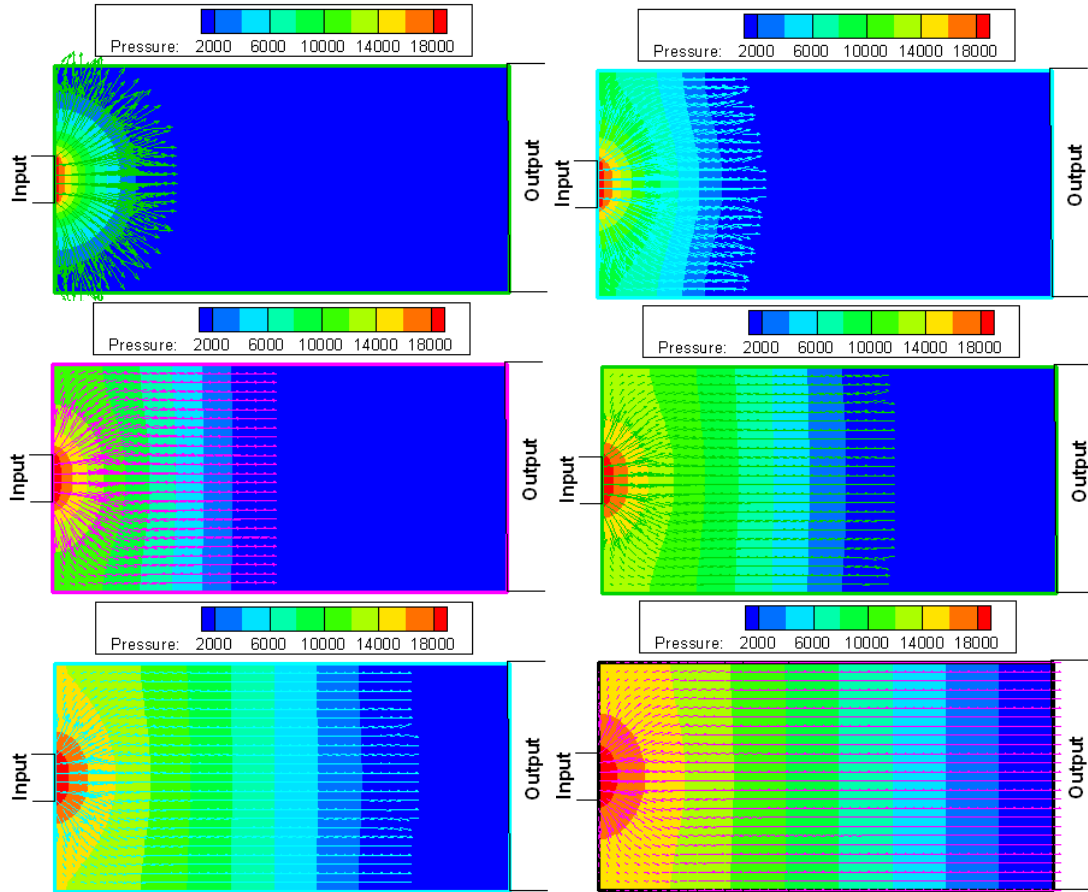


Fig 16 Distribution of Velocity and Pressure in a porous media

3-D Square Geometry Results:

Geometry, Grid and Boundary Conditions: Initial pressure $P=20000$

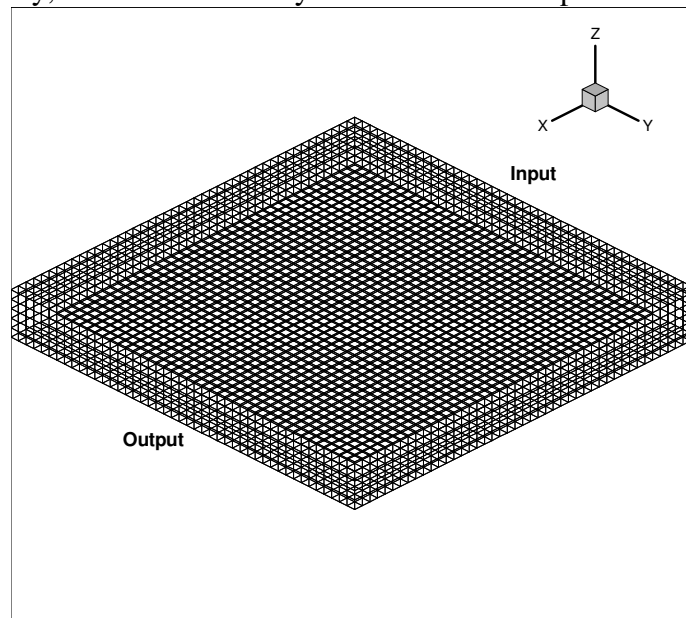
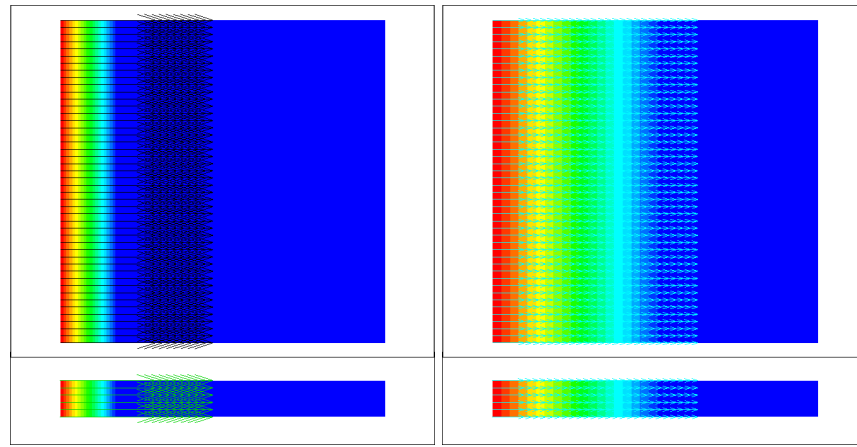


Fig 17 Boundary and Grid



upper map is x-y plane
lower map is y-z plane

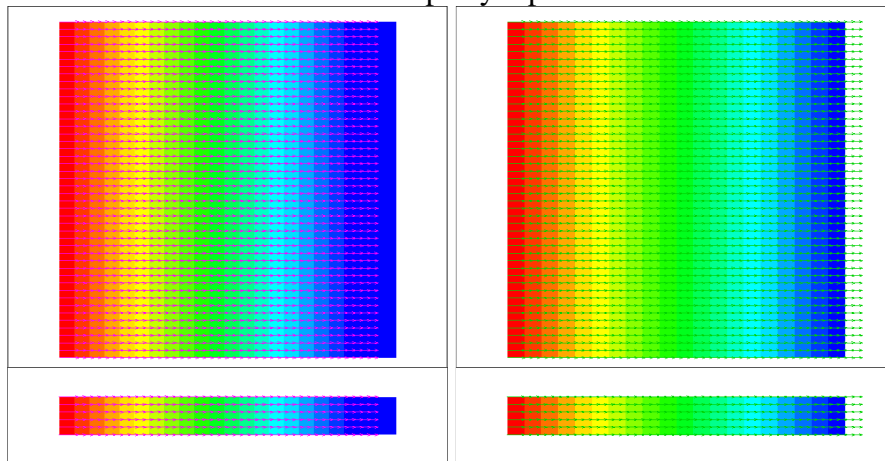


Fig 18 Distribution of Velocity and Pressure in a porous media

3-D Rectangular Geometry Results:
Geometry, Grid and Boundary Conditions: Initial pressure $P=20000$

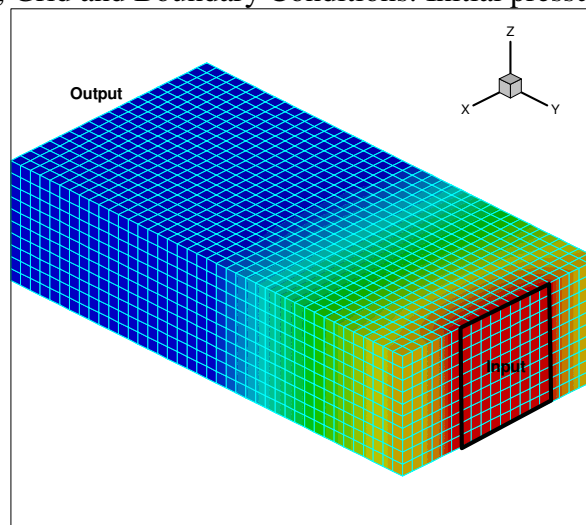


Fig 19 Boundary and Grid

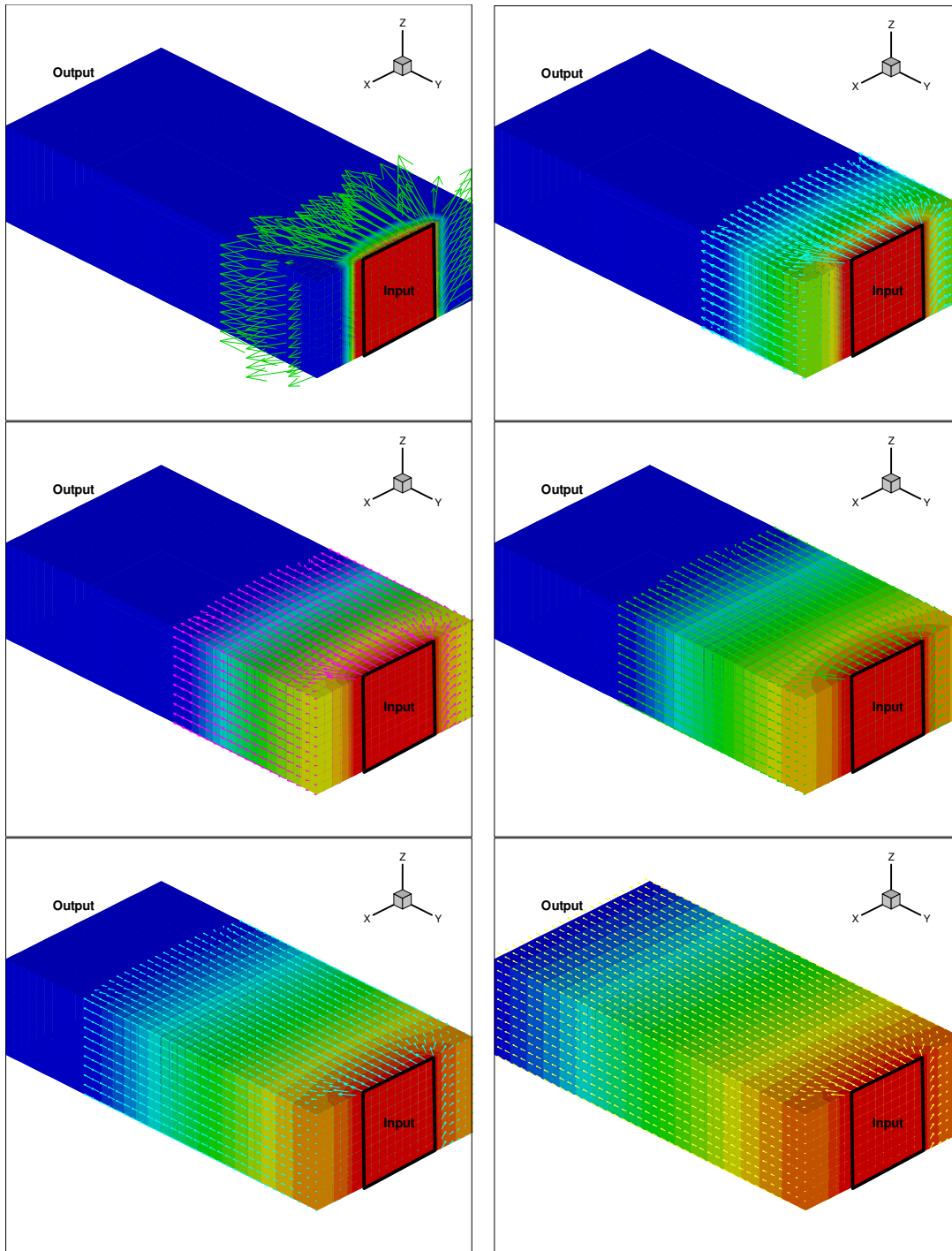


Fig 20 Distribution of Velocity and Pressure in a porous media

10.6 Fast LCM simulation of unsaturated flow in dual-scale fibermats

The problem is a mold of 7"×7" (0.1778×0.1778m) mold that is filling with a resin or a test liquid. The porosity is 0.4742 and the density and viscosity of the liquid are 860 kg/m³ and 0.1875 Pa.s, respectively. The permeabilities of fibermats are 7.303e-10 m² and 6.634e-10 m² along x and y directions and the injection pressure is 20 kPa. We want to study flow of resin in such a dual scale mold. The domain is discretized using FE mesh as shown in Figure 9. For this problem, the Darcy equation and continuity equations are solved to find the pressure distribution using fast LCM mold filling simulation².

The command file is listed as

```

$*****
PORE-FLOW 2D dual-scale flow problem using fast algorithm
$*****
PHYSICAL_PROBLEM
$-----
DARCY_EQUATION: ON
  BODY_FORCES: ON,GX:0., GY:-9.8, GZ:0.
END_DARCY
$-----
FREE_SURFACE: ON
  WICKING: OFF
  DUAL_SCALE:ON
  SINK_MODEL: LUMPED
END_FREE_SURFACE
$-----
END_PHYSICAL_PROBLEM
$*****
PROPERTIES
NUM_OF_SETS=1
$-----
SET 1
  DENSITY: 860
  VISCOSITY: .1875
  POROSITY: .4742
  PERMEABILITY: KX=7.303e-10, KY=6.634e-10, KZ=1e-7, ROTATION=0
  THICKNESS: 1. ! valid for 2D filling analysis
  SINK_FUNCTION: A1=4.25773, A2=1.02833, A3=1.28814, B=19593.45
ENDSET 1
END_PROPERTIES
$*****
MESH_DATA
$-----
DIMENSIONS

```

² For detail about this method, see following paper:

Hua Tan, Pillai, K.M., Fast LCM Simulation of Unsaturated Flow in Dual-Scale Fiber Mats Using the Imbibition Characteristics of a Fabric-Based Unit Cell, Polymer Composites, 31(10), 1790–1807, 2010.

```

NUMBER_NODES: 441
NUMBER_ELEMENTS: 400
SPACE: 2D
ELEMENT_TYPE: QUAD 4
AXISYMMETRY: NO
END_DIMENSIONS
$-----
GEOMETRY
INCLUDE C:\POREFLOW\sourcecode_ver1_01\Mold_Geom_2D.dat
END_GEOMETRY
$-----
END_MESH_DATA
$*****
BOUNDARY_CONDITIONS
$-----
INITIAL_CONDITIONS
VX=0. VY=0. VZ=0.
END_INITIAL
INCLUDE C:\POREFLOW\sourcecode_ver1_01\Mold_BC_2D.dat
$-----
END_BOUNDARY_CONDITIONS
$*****
NUMERICAL_TREATMENT
TIME_DATA: INITIAL_TIME=0.0 FINAL_TIME=5 TIME_STEP_SIZE=1. THETA=0.5
INTEGRATION_POINTS: 4
ITERATION: PICARD
ERROR: 5.D-5
OUT_OF_CORE: OFF
END_NUMERICAL_TREATMENT
$*****
OUTPUT
FILE_NAME: Duel_fast_results.out
FREQUENCY: STEP=20
MUMPS_INFORMATION:Off
END_OUTPUT
$*****

```

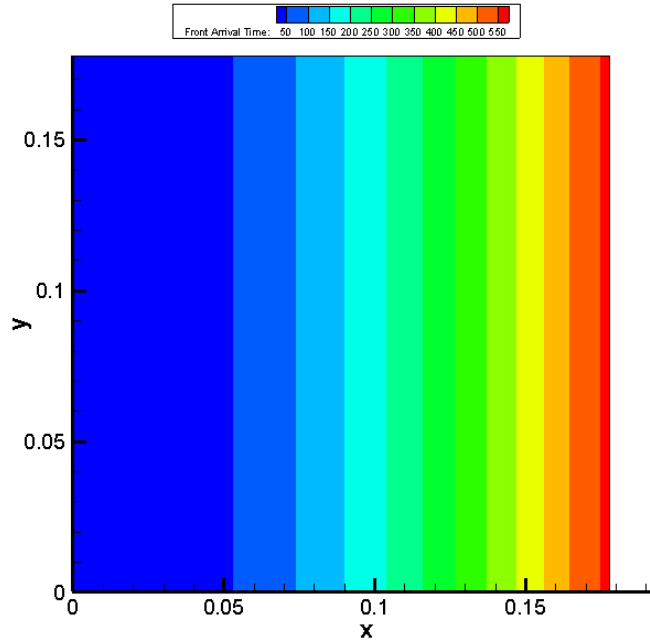


Figure 21: Liquid front movement

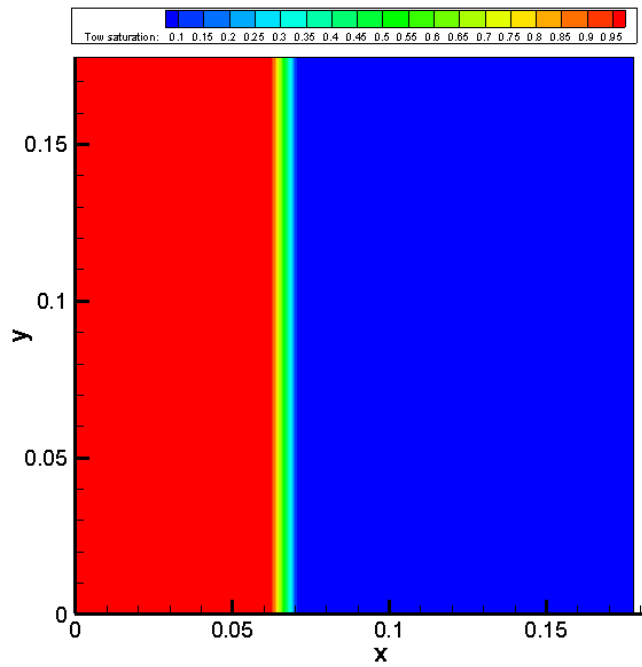


Figure 22: Tow saturation as liquid front moves

10.7 Flow Modeling in a Diaper/Paper

POREFLOW can also model wicking and absorption of liquids into porous substrates. Diapers are porous substances that absorb and retain liquid at a fast rate. The driving force that makes liquid get absorbed by diapers is the capillary pressure. Here we considered a simple block (representing a thick sheet of paper or a section of diaper) of size $20 \times 10 \times 5$ mm with a permeability of 2.34×10^{-9} m² in all directions and a porosity of 0.75. The capillary pressure, which acts on the liquid front, is taken to be 2000 Pa. Here are a series of pictures showing the filling pattern (Blue-wet region, red-dry region):

