A framework for multi-scale three-phase integrated flow-stress process model

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ABSTRACT

The three-phase integrated flow-stress model has been developed at UBC to overcome the drawbacks of the decoupled approach. The flow-compaction and stress-deformation steps are integrated into a unified framework to capture the interplay between different physical phenomena in a seamless manner. The model defines solid displacement, fluid and gas velocity, and fluid and gas pressure (within a $u - v - p$ formulation) as unknowns and solves the system of governing equations using a mixed finite element method with bilinear displacement and velocity shape functions and piecewise constant pressure finite element spaces. However, the current model is not scalable and assumes that the pressure in the two flowing phases are equal.

Experimental results show that the resin impregnation in intra-tow and inter-tow regions occurs at different time-scales. The dual-scale geometry of the fiber-bed results in a lagging flow-front at the micro-scale, entrapment of gas inside the tows, and constant intra-tow permeability upon external pressure. The micro-scale interaction of gas and resin plays a major role in the mentioned observations. This study aims at establishing a framework to extend the current Three-Phase Integrated Flow-Stress Model (3P-IFS) to handle both the local and global physics in their corresponding scales. This paper investigates the capabilities of the current model to be extended to microscale and discusses the data-handling, boundary conditions, and checking processes to assure that the correct physics are captured by the numerical model.

KEYWORDS: Multiscale methods, composite processing, Integrated flow-stress model, Finite Element Analysis

1 INTRODUCTION

The high production cost and the great risk involved in creating a new composites manufacturing process can be significantly mitigated using science-based simulation methods. Moreover, experts argue that use of models can accelerate the certification process and assist process-structure-property optimization. To use a simulation package for manufacturing or certification of a composite part, it should be able to investigate the robustness of each process, which can just be achieved through accounting for all the main phenomena involved during processing. Complicated interconnection of the physical phenomena in composite processing, significant variability of the input parameters, and the significant computational cost of utilizing complex simulation packages are on-going issues in research and industry.

While composites processing has been modelled using sequential independent sub-models for over two decades (Hubert, 1996; Johnston, 1997), the Integrated Flow-Stress (IFS) model for processing of composite materials has been developed recently (Amini Niaki, 2017, Haghshenas, 2012) to tackle the shortcomings of the decoupled approaches. The IFS model calculates the global parameters using a mixed set of phenomenological and physical models through a mixed finite element method with bilinear displacement and velocity shape functions and piecewise constant pressure finite element spaces (Süli, 2013). Experimental data shows that assuming a single-phase porous medium might neglect important dual-scale interactions.

The single-scale porous medium assumption considers the preform to have uniform pre-distribution of pores. This assumption implicitly implies that a phenomenological model for porosity is sufficient to describe the preform and the pores in the preform behind the flow front are fully saturated.

Because of the dual-scale nature of the fibre mats, the resin velocity and pressure in the inter-tow channels are different than the intra-tow channels, which results in the presence of partially-saturated region behind the macroscopic flow front during resin impregnation. The multiscale nature of fabrics has some well-documented influence on mold-filling such as the formation of voids, the creation of a partially saturated region behind the flow-front, and a drop in the inlet-pressure history under the constant injection rate observed in 1D flow experiments (Tan & Pillai, 2012). These observations contradict the fully saturated region assumption behind the flow front.

During composite processing, the configuration of the porous medium will change as a result of consolidation and squeeze flow. This change in configuration is different in each scale. The intra-tow region is compressed enough and cannot be effectively compressed any further, while empty spaces in the inter-tow region can be compressed further to increase the volume fraction of fibers. The dependence of permeability on consolidation can be defined either with a fitting parameter or by rigorous dual scale flow simulations.

Entrapped air inside the preform significantly changes the permeability. The gas and resin flow in the local scale is usually addressed by solving the full Navier-Stokes equation, which is computationally costly. There is a lack of low-order local models that address gas entrapment inside the tows during the flow deformation process. Moreover, many of the investigations also neglected the effect of wicking and capillary suction at the initial stages of impregnation, when the gap pressure is small. The effect of capillary pressure on permeability should be addressed on the local scale.

The temperature gradient in a dual scale medium can affect the local cure and viscosity as well as volatile response. Heat transfer equations should be incorporated into the model to account for those physics. Finally, proper validation test cases should be conducted. The sink term and dual permeability are usually used as fitting parameters while matching the numerical predictions with the experimental results, which make those values dependent on the part shape and the process configuration.

In principle, it would be possible to capture all of the physics at the microscopic scale, but such models are often too complex for the analysis of large structures and produce redundant data. Multiscale modelling is a solution for the abovementioned problems, where microscopic and macroscopic models are coupled to combine the accuracy of microscopic models with the efficiency of macroscopic ones. Thus, the global degrees of freedoms are decreased while the important physics of the process at different scales are preserved.

Different models have been introduced in the literature to account for the dual-scale physics in liquid composite molding (LCM) processes. Tan and Pillai coupled a coarse global mesh and a fine local mesh with periodic 3D unit cells of fabric to simulate the flow under isothermal and non-isothermal conditions (Tan & Pillai, 2012). Kuentzer et al. (Kuentzer, Simacek, Advani, & Walsh, 2006) added 1D elements to each node of a standard 2D or 3D mesh to represent the fibre tows. The delayed impregnation of the intra-tow region is included as sinks of resin in the macroscopic flow field and the global continuity equation has been modified to include a non-zero sink term, which is defined as a function of the rate of saturation. Lawrence et al. (Lawrence, Neacsu, & Advani, 2009) built on top of the abovementioned model and included the effect of capillary pressure as the boundary condition for the 1D element.

The current paper aims to establish a framework for connecting the the current global-scale IFS model to a local-scale model. In the next section, the governing equations of the IFS model are presented. Subsequently, in order to address the scalability of the model, an ABAQUS *UserElement* is developed. The shortcomings of the assumptions and available features of the *UserElement* directed us to an Open Source FE package, FEniCS. The same model is implemented in this package and results are discussed. Finally, a framework for connecting global- and local-scales is introduced and discussed.

2 INTEGRATED FLOW-STRESS MODEL FORMULATION

The two-phase system considers a compressible fluid phase flowing through a porous medium. The governing equations for this problem, including mass and momentum conservations of the system, and Darcy's law creates a system of partial differential equations. While the full form of the equations, including the free strain terms and solidification factor, is provided in (Amini Niaki, 2017), we are using a simplified version here which captures the necessary interactions between the two phases.

$$\boldsymbol{\nabla}\cdot\frac{\boldsymbol{\partial u}}{\boldsymbol{\partial t}}+\boldsymbol{\nabla}\cdot\left(\boldsymbol{v}_f^d\right)+\left(1-\varphi_f\right)\frac{\dot{\langle\rho_s\rangle^s}}{\langle\rho_s\rangle^s}+\varphi_f\frac{\dot{\langle\rho_f\rangle^f}}{\langle\rho_f\rangle^f}=0 \quad (1)$$

$$\nabla P_f=-\frac{\mu}{k}\boldsymbol{v}_f^d \quad (2)$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}=\boldsymbol{0} \quad (3)$$

In the above equations, s and f indices show the solid and fluid properties, $\langle\rho_i\rangle^i$ is the intrinsic average density of phase i, $\boldsymbol{u}$ is the displacement of the solid, $\boldsymbol{v}_f^d$ is the Darcy velocity of the fluid phase, φ_f and P_f are the volume fraction and pressure of the fluid. Moreover, $\boldsymbol{\sigma}$ is the total stress of the system, which can be determined using the Biot's assumption $\boldsymbol{\sigma}=\boldsymbol{\sigma}'-bP_f\boldsymbol{I}$. The Biot's coefficient b is a representation of the compressibility of the solid medium with respect to the grains. The effective stress is described using the solid constitutive model.

2.1 Three-phase model

The three-phase model has also been developed and elaborated in (Amini Niaki, 2017; Niaki, Forghani, Vaziri, & Poursartip, 2018). However, the interaction between the two flowing phases is not yet established properly and should be described as an additional equation involving the relationship between the pressures of the two fluids. The simplest form assumes the difference between the two pressures to be a function of the geometry of the contacting surfaces. At the micro-scale, Lawrence et al. (Lawrence et al., 2009) argued that the bubble entrapment can be modelled using the same procedure. When all the air escapes through the resin, resin replaces the empty region inside the tows with no resistance. Thus, the pressure inside the tow will remain constant and equal to the difference between the capillary pressure and the vent pressure. When the resin completely entraps the air, the air pressure increases as its volume decreases and the back pressure eventually stops the resin. They used arbitrary curves to change the tow pressure between these two cases based on the local saturation.

3 IMPLEMENTATION

The current IFS model has been implemented in MATLAB. However, it has not been scaled up to solve real-world structures. The scalability issue is due to the lack of tools in MATLAB for creating and meshing complex geometries, the lack of established features such as contact, the difficulty of modifying and creating nonlinear solvers, and significant workload to port the created model to the current commercialized advanced composites process simulation software COMPRO.

This section describes different ways that have been tested to implement the two phase model in an advanced finite element package. In the first section, implementation of the model as an $u-p$ ABAQUS

UserElement is described. Then, the $u-p$ model is compared with the $u-v-p$ model, and finally, implementation of the $u-v-p$ model in another code, FEniCS is discussed.

3.1 $\boldsymbol{u-p}$ *UserElement*

The coupled two-phase model uses a $u-v-p$ element, which has 4 nodes at its corners for the velocity and displacement and one node at the center for the pressure in a quadrilateral element. A new element can be implemented in ABAQUS using the user-defined elements (*UserElement*). In an ABAQUS *UserElement*, we can modify the degrees of freedom as necessary. Thus, we used the degree of freedom #11 to represent the fluid pressure and created a $u-p$ model. In the $u-p$ formulation of the IFS model, the velocity is calculated in the post-processing step, using the pressure field and Darcy's law.

A benchmark problem in porous media is the 1D consolidation with a drained top surface, which has an analytical solution (Verruijt, 2013). The top surface is drained, while the bottom and side surfaces are impermeable. Pressure is applied at the start of the analysis and the column is analyzed to obtain the equilibrium state. The geometry and properties of the column are shown in Figure 1.

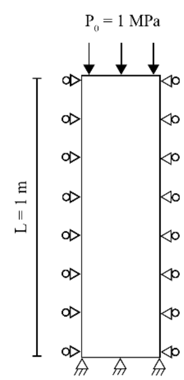


Table 1: Material properties of the column

Material Parameters	Value
Young Modulus ($\boldsymbol{E}$)	$100.0\ MPa$
Poisson's Ratio ($\boldsymbol{\nu}$)	0.25
Permeability ($\boldsymbol{k}$)	$8.0 \times 10^{-14} m^2$
Dynamic viscosity ($\boldsymbol{\mu}$)	$1.0 \times 10^{-5} Pa.s$

$$\bar{p} = \frac{p}{p_0} \text{ (normalized pressure)}$$

$$\bar{x} = \frac{x}{L_0} \text{ (normalized distance)}$$

Figure 1: Geometry and material properties used in modelling the consolidation of a 1D porous medium (column)

In order to compare the pressure at different points in time, L_0 is considered to be the undeformed length of the column. The solution of *UserElement* is compared with the analytical solution in Figure 2 (left). The normalized time is defined as $\bar{t} = \frac{t}{T_0}$, where T_0 is a unit second. The deformation and the contour of pore pressure of the column are shown in Figure 2 (right), which clearly shows the deformation (not to scale) and the dissipation of pressure in time.

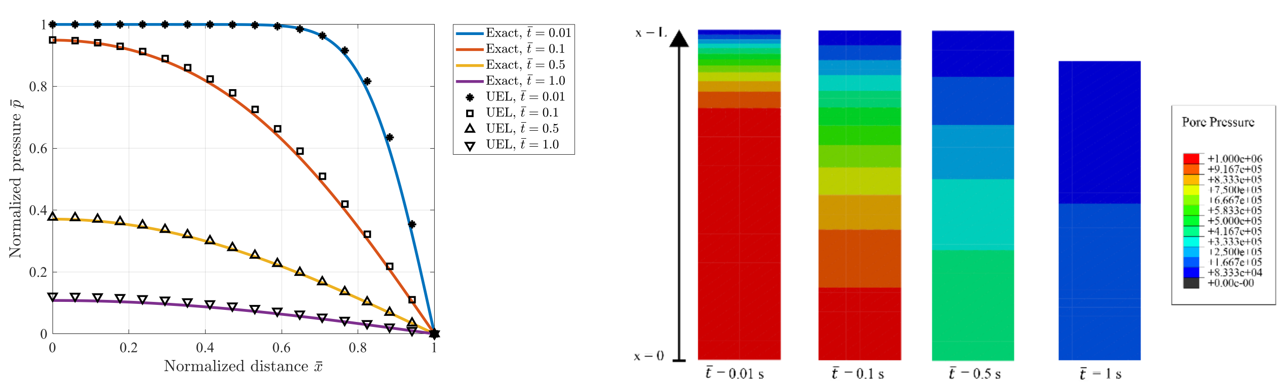


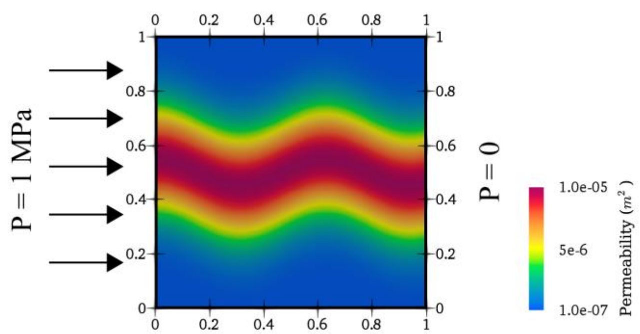
Figure 2: Comparison of analytical and numerical results for column consolidation (left), and the pore pressure and deformation of the column at different points in time (right)

The Darcy's law requires the shape functions of pressure to be an order higher than velocity. Moreover, it can be shown that the Discontinuous Galerkin element of zeroth order cannot capture the pressure gradient effectively in a coupled analysis (Kanschat & Rivière, 2010). While the ABAQUS implementation enforces the conservation at the global scale, post processing the velocity does not enforce mass conservation strongly (i.e. it does not satisfy the differential equation for conservation of mass). In the following section, two methods are compared in order to quantify the effect of spurious sink or source terms.

3.2 Mixed formulation and divergence conforming elements

As mentioned before, solving the flow-compaction equation by eliminating the velocity (i.e. in the Poisson's form), demands the velocity to be calculated in the post processing step. The calculated velocity does not satisfy the conservation equation locally (at the element level), which results in spurious source and sink terms. If the continuity equation is included in the system of equations and matching function spaces are used for velocity and pressure, the mass conservation will be enforced weakly in each element. However, a divergence conforming $H^{div}(\Omega)$ space will enforce the mass conservation strongly, meaning the divergence of velocity is pointwise zero inside the mesh cells. Raviart-Thomas elements are divergence conforming and have been tested extensively for the simulation of coupled Darcy flows (Kanschat & Rivière, 2010).

In order to quantify the effect of weakly enforced mass conservation, the flow inside a rigid porous medium with the spatial change of permeability is modeled using Darcy's law and mass conservation in the Poisson's form $(-\frac{k}{\mu}\boldsymbol{\Delta}P = 0)$ and mixed form $(p - v)$. The geometry of the problem and the permeability of the medium are shown in Figure 3.



$$\begin{cases} -\frac{k}{\mu}\boldsymbol{\nabla}P = \boldsymbol{v} \\ \boldsymbol{\nabla}\cdot\boldsymbol{v} = 0 \end{cases} \quad in \quad \Omega = [0,1]^2$$

$$BC: P = 1 - x \; for \; (x,y) \in \partial\Omega$$

$$k = \max\left\{10^{-5} e^{-\left(\frac{y-0.5-0.05\cos(10x)}{0.2}\right)^2}, 10^{-7}\right\} m^2$$

$$\mu = 10^{-5} \; Pa.s$$

Figure 3: The permeability field on the unit square geometry used for comparison of errors

The problem is simulated using different mesh sizes. The results obtained from a 64×64 mesh are shown in Figure 4. As is clear from Figure 4 (right), the magnitude of velocity between the two methods can vary up to 3%. In order to get a better understanding of the dependency of error in velocity for different mesh sizes, the least-square error is compared in Table 1, which shows a linear reduction in error as we refine the mesh.

Table 2: Least square error in velocity in different mesh configurations

	8×8	16×16	32×32	64×64	128×128
Error	0.0926	0.0480	0.0242	0.0121	0.0060

The mass conservation is very important when the solution is passed to the microscale. Small errors in the global scale might have a significant effect on the microscale calculations. The next section describes the implementation of the IFS model in an open-source finite element package with valuable numerical analysis tools to capture the physics.

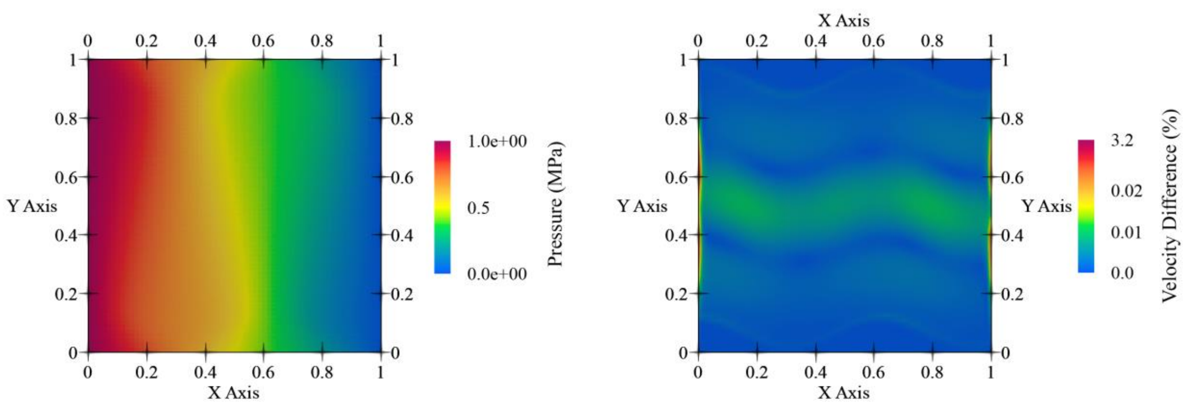


Figure 4: The pressure field using mixed method (left) and the difference in velocity between the two methods (right)

3.3 FEniCS implementation

FEniCS is an open-source computing platform for solving partial differential equations with a library of elements, a remarkable potential to tackle multi-phase problems with mixed spaces, and parallel processing capabilities. Since we showed the benefits of using mixed elements in the flow problem, we are interested in implementing the IFS model in FEniCS. While FEniCS has powerful capabilities in assembling and solving any system of PDEs, other parts of the problem, including complex material models in composite laminates, has to be implemented.

In this section, a simple orthotropic material model for the porous solid is coupled with a non-solidifying single-phase fluid. The angle-laminate geometry (Haghshenas, 2012) is used as a case-study. The material properties and micromechanics model is adopted from (Amini Niaki, 2017). Nonlinear elasticity model of fibers and viscoelastic behavior of resin are not yet implemented for simplicity. Also, the volume fraction is not updated as draining takes place and is kept constant at 42% at all times. The load is applied as a ramp for the whole analysis time, which is 200 minutes. The top and left surfaces are permeable, while the bottom and right surfaces are impermeable. Since all of the details are not implemented in this model, the results are considered as qualitative representation for the time being.

The displacement contours in Figure 5 (right) show the corner-thickening. The pressure distribution in Figure 6 (left) shows that the loading is transferred to fluid pressure at the impermeable surface, while the permeable surface maintains the pressure as specified by the boundary condition ($p = 0$). Also, the velocity magnitude in Figure 6 (right) shows the fluid flux out of the system through the right boundary.

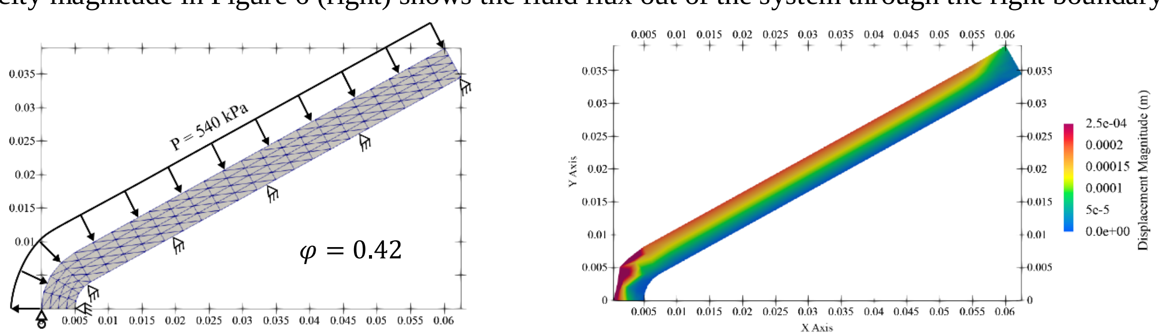


Figure 5: The geometry and loadings (left) adapted from (Haghshenas, 2012), and the predicted displacement magnitude (right) at the end of the loading step

As shown in this case-study, the FEniCS implementation provides promising results for the IFS model. The implemented elements and modules in this package, while enhancing the accuracy and reliability of the results, enable us to add new features to the current model. As mentioned in the introduction, multiscale analysis of the manufacturing process provides new opportunities to include inter-tow physics in the model. The following section briefly discusses a framework for this purpose.

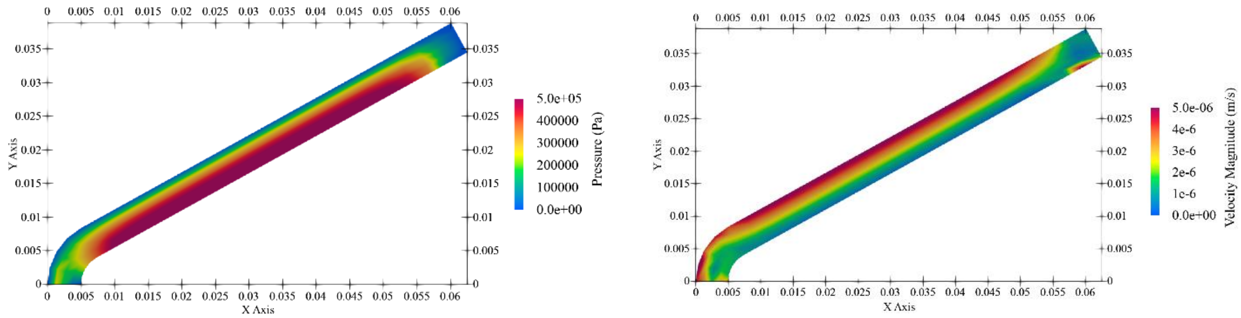


Figure 6: The pressure contours (left), and the velocity distribution (bottom-right) at the end of the loading step

4 MULTISCALE FRAMEWORK

The linking between different scales in a multi-scale problem can be established in different ways (Kanouté et al. 2009). The assumption for the macro- and micro-scale as well as the link between these two should emphasize the distinguishing and important physics at each scale.

The presented multiscale framework, graphically represented in Figure 7, has the following properties:

1. The scales are coupled through transferring boundary conditions. At each time-increment, the macro-scale model is solved using the global mesh while the micro-scale model is solved in the activated elements.
2. The microscale model is activated for elements with two fluid phases and when the element is completely saturated, the microscale model will be deactivated.
3. The macro-scale model includes the flow-compaction, stress-deformation, and heat-transfer physics, while the microscale model just considers the flow and capillary effects.
4. The inter-tow flow of resin is modelled as added sink terms to the local mass conservation
5. The capillary pressure and gas captivation is modelled as a pressure boundary condition applied to the local elements.

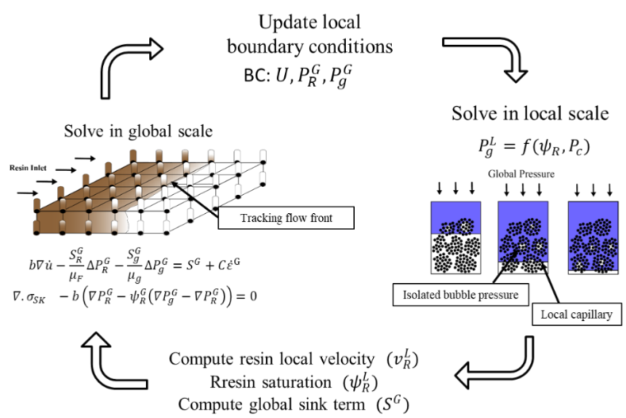


Figure 7: The multiscale framework for coupling inter-tow and intra-tow physics

5 CONCLUSION

This paper discusses the possibility to add multi-scale physics to the current integrated flow-stress (IFS) model for process simulation of composites. The multi-scale properties of the fiber bed result in small-scale physics that cannot be captured in the global domain. In order to simulate capillary effects, consolidation-dependent permeability, and gas captivation, as well as their effect on the global response of the structure during processing, an effective and efficient multi-scale model should be developed. The first part of this paper discusses the methods to implement and extend the current model within sophisticated finite element packages. Two common formulations for flow in an elastic porous medium are compared and the higher accuracy of a divergence conforming Darcy flow formulation is demonstrated. The second part of this paper demonstrates the capabilities of an open-source finite element package in handling the IFS formulation and provides a preliminary framework for adding micro-scale physics to the current model. The desired properties of a multiscale IFS model are highlighted and a framework for implementing those physics is proposed. Work is currently underway by the authors to develop the multi-physics, multi-scale finite element framework and use it to predict the response of real-world composite processing experiments.

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