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RESEARCH ARTICLE

Thixoviscoplastic flow simulations based on Houska thixotropic and Bingham viscoplastic models

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Abstract
We present finite element method (FEM) simulations for quasi-Newtonian modeling approach for thixoviscoplastic (TVP) flow problems. TVP flows are based on Houska thixotropic and Bingham viscoplastic models, which leads to coupled multifield nonlinear problems, which requires on the one hand efficient solver, and a delicate treatment of boundary conditions (BCs) on the other hand. We use FEM monolithic adaptive discrete Newton-multigrid method with efficient FEM discretization choice, that is, discontinuous linear pressure and biquadratic for both velocity and microstructure. In regard to BCs settings, we concretize our analysis for channel flow configuration, and develop one-dimensional reduced model assuming fully developed flow, which provide us with discrete data that we use as BCs and validation tool for two-dimensional FEM simulations.

1 | INTRODUCTION

Numerical simulations of thixoviscoplastic (TVP) flow problems constitute a concrete example of the symbiosis relation of applied mathematics and applied mechanics, which we represent with the double cycles chain process in Figure 1. Examples of thixotropic materials include both natural and the engineered ones, as for instance, gelatin, concrete, aqueous iron oxide or pectin gels, waxy crude oil, carbon black suspension in molten tire rubber, colloidal suspensions. Thixotropic phenomena can be encountered in many industrial processes of real-life applications, namely mixing or transporting material inhabiting thixotropy. Houska thixotropic and Bingham viscoplastic models are the backbones of TVP constitutive equations, which require efficient numerical methods and practical algorithmic tools for its solutions in different circumstances, as for instance geometries and boundary conditions (BCs), encountered in complex fluidic processes. The modeling approach we are considering for Bingham yield stress materials is of quasi-Newtonian type as a straightforward choice to generalize finite element settings of Navier-Stokes equations. For yield stress materials, quasi-Newtonian modeling approach uses modified semi-norm of shear rate with a regularization parameter [1, 2]. For Houska thixotropic model, as a simple modification of Bingham viscoplastic model using microstructure as an additional field, it incorporates the internal material microstructure via microstructure dependent viscosity. Consequently, the plastic viscosity and the yield stress are microstructure dependent. Furthermore, the generalized Navier-Stokes equations are upgraded with microstructure equation which encompasses the thixotropic models via the interplay of buildup, and breakdown functions representing the aging, and rejuvenation phenomena of thixotropic material, respectively, resulting in generalized TVP Navier-Stokes equations.

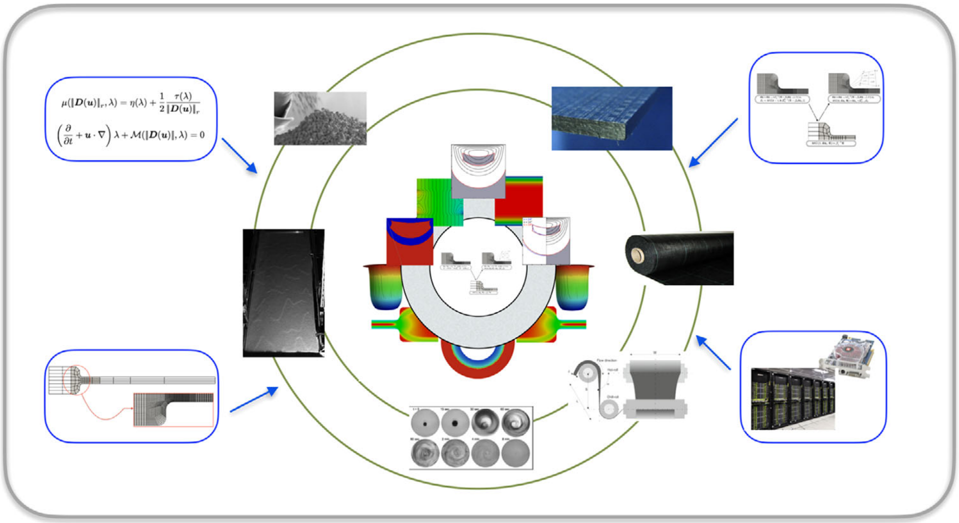

FIGURE 1 Applied mathematics and applied mechanics merging for the simulations of complex fluidic processes.

Generalized TVP Navier-Stokes equations require efficient numerical methods and practical algorithmic tools for its solution due to regularization parameter and the strong nonlinearity. We developed an adaptive combined discrete Newton's/monolithic geometric multigrid solver, it is based on an adaptive step-size in finite difference for discrete Newton's, and Local Pressure Schur Complement (LPSC) to solve simultaneously all fields of the linear problems, which benefit from discontinuous (linear) finite element method (FEM) pressure approximations aspect, and the collocation of the remaining fields in the same d.o.f. in FEM interpolation (quadratic).

We introduce TVP quasi-Newtonian modeling approach, and present the Bingham-Houska TVP problem in a general FEM abstract framework as strongly coupled multifield nonlinear problem in Section 2. Then in Section 3, we analyze the important issue of BCs settings for complex yield stress material in channel configuration. We provide an optimal BCs setting for coupled multifield TVP problem via discrete Dirichlet BCs deduced from one-dimensional reduced model assuming fully developed channel flow, which we additionally use for validation of two-dimensional FEM solutions.

2 | TVP QUASI-NEWTONIAN MODELING

The Houska TVP [3] flow simulation problem under investigation uses generalized viscosity $\mu(\cdot,\cdot)$ function dependent on microstructure λ, and shear rate approximation, $D_{\mathbb{I},r}$ [4],

$$\mu(D_{\mathbb{I},r},\lambda) = \eta(D_{\mathbb{I},r},\lambda) + \tau(\lambda)\frac{\sqrt{2}}{2}\frac{1}{\sqrt{D_{\mathbb{I},r}}}, \tag{1}$$

$\eta(\cdot,\cdot)$ denotes plastic-viscosity, $\tau(\cdot)$ is the yield stress. Also, we use the shear rate approximation, $D_{\mathbb{I},r}$ for the breakdown $\mathcal{F}(\cdot,\cdot)$, buildup $\mathcal{G}(\cdot,\cdot)$. Furthermore, Houska model functions are defined as follows:

$$\begin{cases} \eta(D_{\mathbb{I},r},\lambda) = \eta_0 + \eta_\infty\lambda, \\ \tau(D_{\mathbb{I},r},\lambda) = \tau_0 + \tau_\infty\lambda, \\ \mathcal{F}(D_{\mathbb{I},r},\lambda) = \mathcal{M}_a(1-\lambda), \\ \mathcal{G}(D_{\mathbb{I},r},\lambda) = \mathcal{M}_b\lambda\sqrt{D_{\mathbb{I},r}}. \end{cases} \tag{2}$$

We used an approximation for Forbenius norm of symmetric part of velocity gradient. Here η_0, and τ_0 are plastic viscosity and yield stress in absence of thixotropy, respectively. η_∞, and τ_∞ are plastic viscosity, and yield stress related to the microstructure. The buildup, and breakage constants are denoted by $\mathcal{M}_a$, and $\mathcal{M}_b$, respectively.

The system of set equations for TVP flow is given as follows [5]:

$$\begin{cases} \left(\frac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla\right)\boldsymbol{u} - \nabla\cdot\left(2\mu(D_{\mathbb{I},r},\lambda)\mathbf{D}(\boldsymbol{u})\right) + \nabla p = \boldsymbol{f}_{\boldsymbol{u}}, \\ \nabla\cdot\boldsymbol{u} = 0, \\ \left(\frac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla\right)\lambda - \mathcal{F}(D_{\mathbb{I},r},\lambda) + \mathcal{G}(D_{\mathbb{I},r},\lambda) = f_\lambda, \end{cases} \tag{3}$$

in Ω, with external forces $\boldsymbol{f}_{\boldsymbol{u}}$, and f_λ. The boundary $\partial\Omega$ have an inflow Γ^-, outflow section Γ^+ sections, and $\Gamma = \Gamma^- \cup \Gamma^+$. $\boldsymbol{u}$, p, and λ denote velocity, pressure, and microstructure, respectively.

We introduce the spaces $\mathbb{V} := (H_0^1(\Omega))^2, \mathbb{T} := H_{\Gamma^-}^1(\Omega), and \mathbb{Q} := L_0^2(\Omega)$, associated with the norms $\|\cdot\|_{\mathbb{V}}$, $\|\cdot\|_{\mathbb{T}}$, and $\|\cdot\|_{\mathbb{Q}}$, respectively [6, 7]. To write the problem in the operator form, we introduce the dual spaces $\mathbb{V}'$, $\mathbb{T}'$, $\mathbb{Q}'$, and $\mathbb{W}' := \mathbb{V}' \times \mathbb{T}'$, of spaces $\mathbb{V}$, $\mathbb{T}$, $\mathbb{Q}$, and $\mathbb{W} := \mathbb{V}\times\mathbb{T}$, respectively [8]. For the field $\boldsymbol{u}\in\mathbb{V}$, $\lambda\in\mathbb{T}$, and $p\in\mathbb{Q}$, we denote $\tilde{\boldsymbol{u}} = (\boldsymbol{u},\lambda)$, and consider the abstract form of the problem as follows:

Find $(\tilde{\boldsymbol{u}}, p) \in \mathbb{V}\times\mathbb{T}\times\mathbb{Q}$, *such that*

$$\begin{cases} \mathcal{A}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})\tilde{\boldsymbol{u}} + \mathcal{B}^{\mathrm{T}} p = l_{\tilde{\boldsymbol{u}}} & \text{in } \mathbb{V}'\times\mathbb{T}', \\ \mathcal{B}\boldsymbol{u} = 0 & \text{in } \mathbb{Q}'. \end{cases} \tag{4}$$

The problem (4) is coupled thought velocity and pressure $(\boldsymbol{u}, p)$, and velocity and microstructure $(\boldsymbol{u},\lambda)$, with different kind of nonlinearities. The operator $\mathcal{A}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})$ comes apart as follows:

$$\mathcal{A}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})\tilde{\boldsymbol{u}} := \mathcal{A}_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})\boldsymbol{u} + \mathcal{A}_\lambda(\tilde{\boldsymbol{u}})\lambda. \tag{5}$$

We introduce the TVP operators $\mathcal{A}_{\boldsymbol{u}} : \mathbb{V}\times\mathbb{T}\times\mathbb{V} \longrightarrow \mathbb{V}'$, and $\mathcal{A}_\lambda : \mathbb{V}\times\mathbb{T}\times\mathbb{T}\longrightarrow\mathbb{T}'$ as follows:

$$\langle\mathcal{A}_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})\boldsymbol{u},\boldsymbol{v}\rangle = \int_\Omega 2\mu(D_{\mathbb{I},r},\lambda)\mathbf{D}(\boldsymbol{u}) : \mathbf{D}(\boldsymbol{v})\, d\Omega \quad \forall\boldsymbol{u},\boldsymbol{v}\in\mathbb{V},\lambda\in\mathbb{T}, \tag{6}$$

$$\begin{aligned} \langle\mathcal{A}_\lambda(\tilde{\boldsymbol{u}})\lambda,\xi\rangle &= \int_\Omega \left(-\mathcal{F}(D_{\mathbb{I},r},\lambda) + \mathcal{G}(D_{\mathbb{I},r},\lambda)\right)\xi\, d\Omega \\ &- \int_\Omega \lambda\, \boldsymbol{u}\cdot\nabla\xi\, d\Omega + \int_{\Gamma^+} |\boldsymbol{u}\cdot\boldsymbol{n}|\,\lambda\,\xi\, d\sigma \quad \forall\lambda,\xi\in\mathbb{T},\boldsymbol{u}\in\mathbb{V}, \end{aligned} \tag{7}$$

and, the linear forms $\mathcal{B} : \mathbb{V}\longrightarrow\mathbb{Q}'$, $l_{\boldsymbol{u}} : \mathbb{V}\longrightarrow\mathbb{R}$, and $l_\lambda : \mathbb{T}\longrightarrow\mathbb{R}$ as follows:

$$\langle\mathcal{B}\boldsymbol{u},q\rangle = -\int_\Omega \nabla\cdot\boldsymbol{u}\, q\, d\Omega \quad \forall\boldsymbol{u}\in\mathbb{V}, q\in\mathbb{Q}, \tag{8}$$

$$l_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{v}}) = \int_\Omega \boldsymbol{f}_{\boldsymbol{u}}\boldsymbol{v}\, dx + \int_\Omega f_\lambda\,\xi\, d\Omega \quad \forall\tilde{\boldsymbol{v}}\in\mathbb{V}\times\mathbb{T}. \tag{9}$$

We proceed with the simulation of TVP channel flow, and the analysis of the corresponding BCs settings in Section 3.

3 | APPLICATION TO TVP CHANNEL FLOW

The focus of this section is to accentuate the important aspect of the BCs settings for TVP flow simulations. To do so, we simulate Bingham-Houska TVP flow problem in a channel configuration with an inflow Γ^-, and outflow Γ^+ sections subject to inflow, and outflow BCs. We apply adaptive discrete Newton combined with coupled geometric Multigrid method to solve the TVP equation (4). For FEM discretization, we use the stable Stokes FEM pair approximations, that is, biquadratic for velocity, and linear discontinuous for pressure Q_2/P_1^{disc}, and we collocate the microstructure with the velocity d.o.f.

$$u = \begin{cases} \frac{1}{8}\left((1-2\tau_0)^2 - (1-2\tau_0-2y)^2\right) & \text{if } y \in [0, \frac{1}{2}-\tau_0) \\ \frac{1}{8}(1-2\tau_0)^2 & \text{if } y \in [\frac{1}{2}-\tau_0, \frac{1}{2}+\tau_0] \\ \frac{1}{8}\left((1-2\tau_0)^2 - (2y-2\tau_0-1)^2\right) & \text{if } y \in (\frac{1}{2}+\tau_0, 1] \end{cases}$$

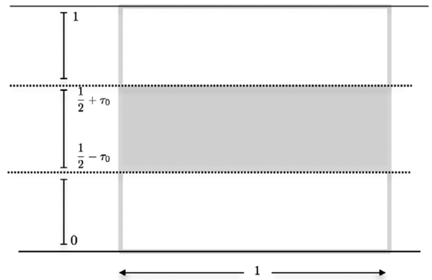

FIGURE 2 Analytic Bingham viscoplastic benchmark: Yield-stress dependent analytic Bingham viscoplastic solution on unit channel, and the corresponding unyielded region located along the center of the channel.

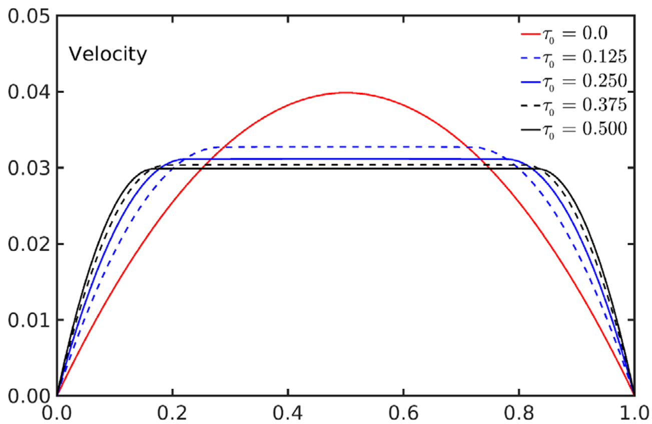

FIGURE 3 Analytic Bingham viscoplastic benchmark: Velocity solutions at, $y = 0.5$ with respect to yield-stress parameter τ_0.

in order to benefit the solver from the velocity-pressure coupling [9]. In regard to strong nonlinearity and coupling of the system of equations, we use adaptive discrete Newton's combined geometric multigrid method, it uses an adaptive step-size in finite difference for discrete Newton's methods, and LPSC schemes to solve simultaneously for all fields of the linear problems.

We start with the classical exact Bingham viscoplastic benchmark on a unit channel, which necessitates the imposing of Dirichlet BCs, to move on to the natural BCs for channel flow with an inflow and outflow sections. Then, we upgrade the Bingham viscoplastic benchmark to include Houska thixotropic model.

3.1 | Bingham viscoplastic channel flow

The classical exact Bingham viscoplastic benchmark consists of a yield stress dependent analytic function $\boldsymbol{u}_{ex} = (u, 0)^{\mathrm{T}}$ on unit channel Figure 2, leading to a unyielded region located along the center of the channel with the width dependent on yield stress parameter τ_0, that is, $y \in [\frac{1}{2} - \tau_0, \frac{1}{2} + \tau_0]$.

We start by performing the numerical simulations by varying yield stress parameter, and use Dirichlet BCs settings as it is given by the analytic function Figure 2, and we set the plastic-viscosity $\eta_0 = 1.0$. We provide the corresponding velocity solution across the line $y = 0.5$ in Figure 3.

Clearly from Figure 3, for the highest value of yield stress $\tau_0 = 0.5$, the unyielded region take over almost full channel. Furthermore, the solutions on yielded regions correspond to Poiseuille law, that is, $\nabla\ p = (-1, 0)^{\mathrm{T}}$.

Next, we provide for one value of yield stress parameter the flow fields solution in Figure 4. A close look on the solutions on the unyielded region reveals that Dirichlet BCs settings leads to a constant pressure, with the clear artifact of the regularization at interfaces between yielded and unyielded regions at inflow and outflow boundary sections in Figure 4 (TOP). To have the Poiseuille flow on both regions, yielded and unyielded, we alternatively apply pressure drop BCs in Figure 4 (BOTTOM).

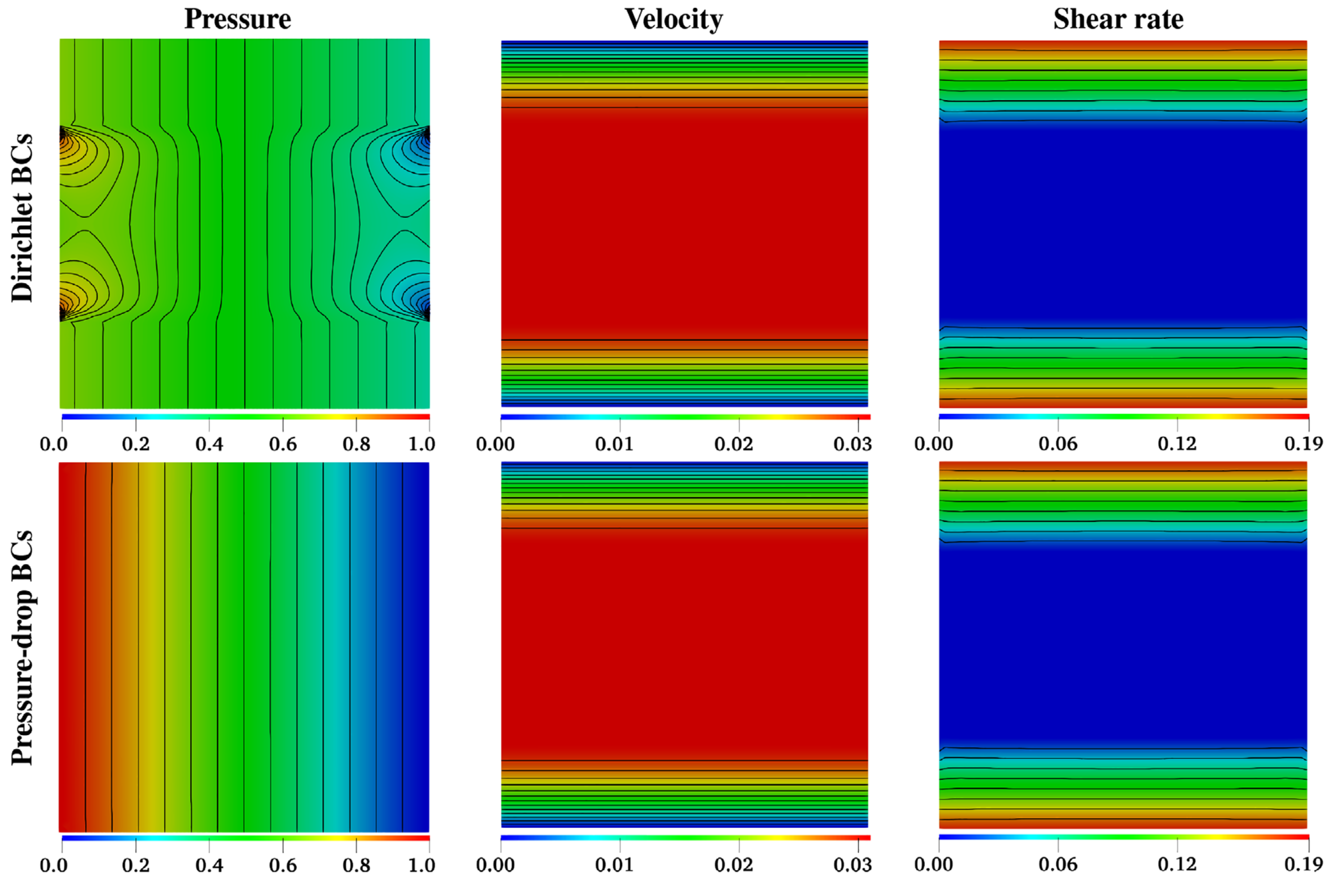

FIGURE 4 Bingham viscoplastic BCs for channel flow: Flow solutions for Dirichlet and pressure drop BCs, where $\eta_0 = 1.0, \tau_0 = 0.25$, $k = 10^4$. BCs, boundary conditions.

Figure 4 shows that with the pressure drop BCs we get rid of the of regularization artifact observed for Dirichlet BCs. Furthermore, to remain with the unidirectional flow assumptions and to remove the well-known reverse flow caused by "do-nothing" BCs [10, 11], we simply set y-velocity to zero. For both BCs settings, Dirichlet and pressure drop, the velocity and shear rate are in perfect agreement with the Bingham viscoplastic solution Figure 2. It is worth to note that the Bingham viscoplastic gives also the condition that the magnitude of shear stress is less than the yield stress parameter on the unyielded region.

Bingham viscoplastic flow evokes the choice of the natural BCs for channel flow for yield stress materials. Since Houska TVP model is an upgrade of Bingham viscoplastic model with microstructure equation, we proceed accordingly to provide the optimal BCs settings for velocity and microstructure for Houska TVP channel flow.

3.2 | TVP channel flow

The microstructure equation in TVP channel flow requires Dirichlet BCs at the inflow section Γ^-. Consequently, we assume fully developed flow conditions for channel flow and develop one-dimensional reduced Houska TVP model. Solving one-dimensional Houska TVP problem provides us with the necessary Dirichlet data in a discrete form for the microstructure, and a validation tool for two-dimensional Houska TVP solutions for all fields. Furthermore, we can use the solutions of one-dimensional model as a Dirichlet data for velocity at inflow and outflow sections. To do so, we provide an alternative remedy for the effect of the well known do-nothing BCs.

In Figure 5, we provide the comparison of the one-dimensional reduced Houska TVP microstructure solution with two-dimensional FEM fully developed solution at cross section $y = 0.5$, and the microstructure flow field.

Clearly, the microstructure flow field distribution along the channel corresponds to the one-dimensional reduced Houska TVP microstructure solution, which confirm the validity of the two-dimensional solution on the one hand, and the

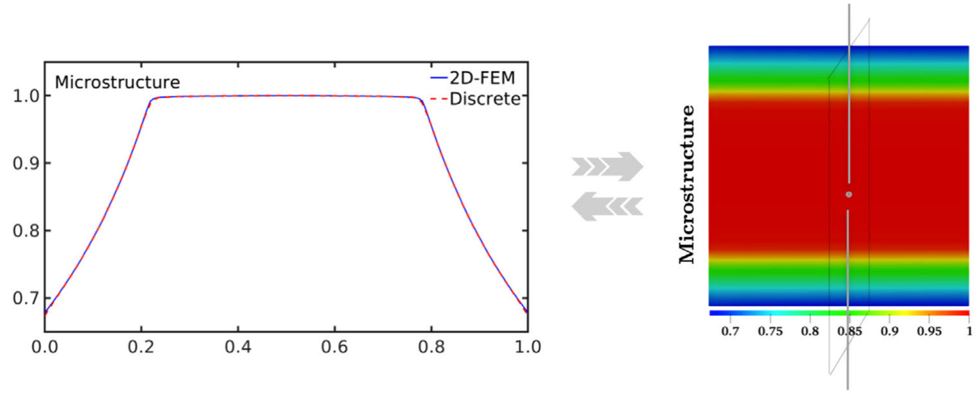

FIGURE 5 Houska TVP fully developed flow: Validation of FEM fully developed 2D microstructure solution with discrete 1D microstructure solution. TVP, thixoviscoplastic.

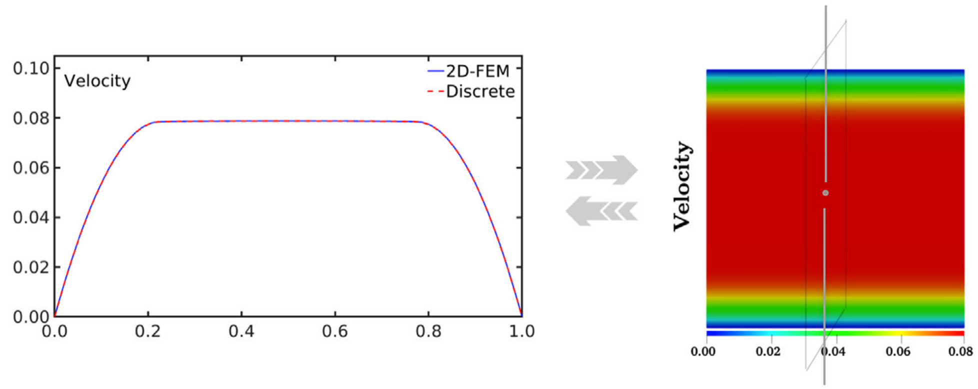

FIGURE 6 Houska TVP fully developed flow: Validation of FEM fully developed 2D velocity solution with discrete 1D velocity solution. TVP, thixoviscoplastic.

fully developed flow assumptions on the other hand. Similarly, Figure 6 displays the comparison of the one-dimensional reduced Houska TVP velocity solution with two-dimensional FEM fully developed ones at cross section $y = 0.5$, and the velocity flow field.

The superposition of the cut line of the velocity solution for two-dimensional FEM fully developed solution at cross section $y = 0.5$ and the one-dimensional reduced Houska TVP, and the distribution of the velocity flow field along the channel confirm the accuracy of the FEM solution, and also the optimal BCs conditions for complex yield stress materials. Moreover, the unyielded zone indicated by microstructure and velocity matches perfectly, confirming once more the efficiency of our numerical methods developed for TVP FEM solver, namely the adaptive combined discrete Newton's/monolithic geometric multigrid, as the quasi-Newtonian modeling approach requires a robust solver w.r.t. regularization.

4 | SUMMARY

In this paper, we investigated the BCs settings for TVP channel flow problem, and presented FEM flow simulations. Our TVP flow is based on Houska thixotropic and Bingham viscoplastic models, and constitutes a multifield nonlinear coupled problem. On the one hand, Bingham-Houska TVP model integrates nonlinearity within momentum and microstructure equations, on the other hand it induces two way coupling. First, we developed one-dimensional reduced Bingham-Houska TVP model assuming fully developed flow to obtain the necessary Dirichlet BCs for the microstructure equation. Second, we used the one-dimensional reduced Bingham-Houska TVP solutions to validate our two-dimensional fully developed FEM solutions. In addition, we provided an optimal alternative remedy for do-nothing BCs for complex yield stress material. The accuracy achieved for our quasi-Newtonian modeling approach for TVP problem confirms the appropriate choice of an adaptive combined discrete Newton's/monolithic geometric multigrid strategy for strongly coupled multifield nonlinear problems.

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