# Improved micro-continuum approach for capillary-dominated multiphase flow with reduced spurious velocity

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Improved micro-continuum approach for capillary-dominated 1 multiphase flow with reduced spurious velocity 2 Zhiying Liu (刘志颖),<sup>1,2</sup> Junyu Yang (杨君宇),<sup>1,2</sup> Qianghui Xu (许强辉),<sup>1,2,3,a)</sup> and Lin Shi (史 3 琳)1,2 4 5 <sup>1</sup>Key Laboratory for Thermal Science and Power Engineering of the Ministry of Education, 6 Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China. 7  $^{2}$ Key Laboratory for CO<sub>2</sub> Utilization and Reduction Technology of Beijing, Beijing 100084, China. 8 <sup>3</sup>School of Mechanical Engineering, Beijing Institute of Technology, Beijing 100081, China. 9 Corresponding author: a) xuqh12@tsinghua.org.cn 10 11 **KEYWORDS** 12 Micro-continuum; Multiscale porous media; Multiphase flow; Spurious velocity; Volume of fluid 13 14 ABSTRACT 15 A diverse range of multiphase flow and transport occurs in multiscale porous media. The 16 multiphase micro-continuum Darcy-Brinkmann-Stokes (DBS) model has been developed to 17 simulate the multiphase flow at both the pore and continuum scales via single-field equations. 18 However, the unacceptable spurious velocities produced by the conventional micro-continuum DBS 19 model present challenges to the modeling of capillary-dominated flow dynamics. This study 20 improves the micro-continuum DBS model to mitigate these spurious velocities at the gas-liquid 21 interface and contact-line regions. A hybrid interpolation scheme is proposed to improve the 22 computational accuracy of the interface curvature and reduce the spurious velocity around the gas-23 liquid interface by 1–2 orders of magnitude. At the porous boundary, the normal to the gas-liquid 24 interface is corrected, and the normal to the solid-fluid interface is smoothed to guarantee the 25 prescribed wettability condition and decrease the spurious velocities at the contact-line region by an 26 order of magnitude. A series of static and dynamic benchmark cases are investigated to demonstrate 27 that the improved DBS model can simulate capillary-dominated multiphase flows with negligible 28 spurious velocities at capillary numbers as low as 10<sup>-4</sup> in both simple and complex geometries. The 29 improved DBS model can combine X-ray computed micro-tomography images to perform 30 multiscale simulations of capillary-dominated multiphase flow and understand the effect of sub-31 resolution porosity on fluid dynamics in naturally multiscale rocks.

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## 34 I. INTRODUCTION

35 Multiphase flows within complicated porous media are widely encountered in many natural and engineering systems, including CO<sub>2</sub> geological sequestration,<sup>1</sup> hydrocarbon recovery,<sup>2, 3</sup> and 36 electrochemical energy systems.<sup>4-7</sup> In these scenarios, multiphase flow and transport are complex 37 38 phenomena, involving strong coupling among inertial, viscous, and interfacial forces in natural geological structures.<sup>8</sup> In the bulk-fluid phases, such as gas and liquid phases, two immiscible fluids 39 40 are separated by an interface, and the interfacial tension strongly influences the shape, movement, 41 and evolution of the phase interface. The viscous force acts tangentially to impede the relative phase 42 motion. In the bulk fluid phases, such as gas and liquid, two immiscible fluids are separated by an 43 interface, where the interfacial tension strongly influences the shape to minimize the interfacial 44 energy. When a fluid of higher density and lower viscosity displaces another fluid of lower density 45 and higher viscosity, the flow process is intrinsically unstable, leading to the fingering of phase 46 interfaces. The porous medium contains considerable fluid-solid interfaces. A contact-line region 47 emerges when the gas-liquid interface joins a solid surface, where the wall-adhesion force governs the contact angle and the contact line dynamics <sup>9</sup>. In the low-capillary flow regime, the gas-liquid 48 49 interfacial force and the wall-adhesion force significantly control the phase evolution and 50 distribution in heterogeneous porous media. A deep understanding of the multiphase fluid dynamics 51 is fundamental for predicting accurate gas, water, or oil fluxes through geological structures and 52 determining the techno-economic feasibility of subsurface engineering techniques.

53 Natural geological structures are typically heterogeneous, multiscale assemblies.<sup>10</sup> Although 54 the porous domain of interest is limited to the millimeter or centimeter scale, the pore space can 55 have length scales covering several orders of magnitude,<sup>11</sup> from micrometer-range pores (~ 56  $O(10) \,\mu\text{m}$ ) to sub-micrometer-range pores (~  $O(100) \,\text{nm}$ ). Multiscale porous structures can be

57 imaged using various imaging modalities, such as X-ray computed micro-tomography (micro-CT), 58 which commonly offers a resolution of a few microns per voxel.<sup>11</sup> With such micrometer-scale 59 resolution, the micrometer-range pores can be resolved to illustrate the void space and the 60 surrounding solid boundary clearly. In contrast, the sub-micrometer-range pores are hidden below 61 the image resolution.<sup>11</sup> The sub-voxel porosity of the unresolved porous medium can be estimated 62 based on the gray intensity, leading to the unresolved porous medium being represented by the effective continuum.<sup>12, 13</sup> The varying representation of porous media at two scales cannot explicitly 63 64 characterize the connectivity of the resolved and unresolved pore space, increasing the difficulty of 65 modeling the multiphase fluid dynamics.<sup>10, 11, 14</sup> Accordingly, two independent mathematical and 66 numerical models are required to adapt the scale-dependent representations of the porous media and 67 account for different multiphase flow physics. The inertial and viscous forces may dominate in the

fully resolved pore space,<sup>15</sup> whereas the multiphase flow can be directly simulated using the Navier-68 69 Stokes equation, referred to as pore-scale modeling, in which the gas-liquid interface is explicitly 70 tracked or captured, and the interface tension force is calculated based on the Young-Laplace law.<sup>16</sup> 71 The capillary force and porous drag force gradually become dominant over the viscous dissipative 72 term within the sub-micrometer-range pores, the result of reduced fluid velocity and intensified 73 solid-fluid friction.<sup>17</sup> Correspondingly, the flow is usually modeled by the multiphase Darcy's law in the unresolved pore medium, referred to as continuum-scale modeling.<sup>14, 16, 18</sup> Different from the 74 75 direct simulation of the inertial, viscous, and interfacial forces in pore-scale modeling, continuum-76 scale modeling prescribes the porosity-dependent and saturation-dependent transport properties of 77 the porous representative elementary volume, including the relative permeability and capillary 78 pressure, to describe the nonlinear relation between the phase-averaging velocity and the driving 79 force.<sup>16, 19-21</sup> Notably, the resolved porous medium coexists with the unresolved porous medium, 80 making it necessary to consider their interaction via appropriate boundary conditions. Therefore, 81 predictive modeling of multiphase flow physics through the inherently multiscale porous medium 82 is highly challenging.

Hybrid-scale modeling is an elegant idea for modeling multiscale flow and transport.<sup>22-29</sup> In 83 84 this approach, single-field equations are introduced to provide a unified framework for describing 85 the scale-dependent physics across the multiscale porous media. This idea dates back to the work of Brinkmann,<sup>30</sup> who proposed the single-phase Darcy-Brinkmann-Stokes (DBS) momentum 86 87 equation. TABLE I lists a brief summary of development and application of the micro-continuum 88 DBS model. In the case of single-phase flow, combining the Brinkmann term with Darcy's law 89 means that the DBS equation remains valid for both the large-scale channel and the porous domain.<sup>17,</sup> 90 <sup>22</sup> Soulaine et al.<sup>14, 18</sup> developed the micro-continuum DBS framework for pore-resolved simulations 91 of single-phase flow. The cornerstone of the micro-continuum framework is the local porosity field 92  $\mathcal{E}$ , which enables adaptation to the multiscale structure. A bounding value of  $\mathcal{E} = 1$  represents the 93 resolved macropores, while a bounding value of  $\varepsilon = 0 \equiv 0.01$  characterizes the impermeable 94 solid,<sup>31</sup> and the intermediate range  $0 < \varepsilon < 1$  describes the unresolved pores. Relying on volumeaveraging theory,<sup>32</sup> the DBS equation solves the standard Navier-Stokes flow in the resolved 95 96 macropore channels, tends asymptotically to Darcy's law in the unresolved porous medium, and 97 reproduces the nonslip velocity condition at the macropore-rock interface by penalization.<sup>15, 16</sup> Many numerical studies have leveraged the micro-continuum DBS framework to demonstrate its 98 99 reliability in modeling single-phase flows across multiscale porous media.<sup>12, 31, 33-35</sup> Scheibe et al.<sup>33</sup> 100 used the DBS equation to simulate flow and transport in 3D micro-CT images with unresolved pores, 101 achieving improved agreement with experimental results. For simulations of reactive flows across 102 a multiscale porous medium, another appealing advantage of the micro-continuum framework lies 103 in its ability to handle the dynamic evolution of the solid-fluid interface without requiring a re-

104 meshing strategy. For example, the mineral dissolution of a single calcite crystal was simulated by Soulaine et al.,<sup>34</sup> and their results agreed with the classic arbitrary Lagrangian-Eulerian solver. Maes 105 106 et al. improved the formulations to localize the reaction at the fluid-solid interface more accurately. 107 They found the micro-continuum DBS framework is significantly faster than the Arbitrary 108 Lagrangian Eulerian (ALE) method for simulations of calcite dissolutions, since the ALE method requires additional treatment for interface displacement.<sup>36</sup> Ashrafizadeh et al. solved the Stokes-109 110 Brinkman and the Poisson-Nernst Planck equations simultaneously to explore the effect of nanochannel shape on the ion transfer behavior.<sup>37, 38</sup> Xu et al.<sup>31</sup> extended the pore-scale micro-111 112 continuum model to non-isothermal reactive flow through a multiscale porous medium. They 113 demonstrated the model improvement in terms of mass and energy conservation compared with the 114 previous lattice Boltzmann methods. Therefore, single-phase fluid dynamics modeling across the 115 multiscale porous medium is well established within the micro-continuum framework, and is widely used in simulations of reactive flow in fractures and mineral precipitation.<sup>35, 39-42</sup> 116

117 The multiphase micro-continuum DBS framework has recently modeled multiphase flows in a 118 multiscale porous medium. Horgue et al.43 and Soulaine et al.14, 18 proposed two-phase micro-119 continuum DBS frameworks by developing a multiphase DBS equation to describe the two-phase 120 flow at both the pore and continuum scales. The DBS multiphase model was reduced to the classic 121 volume-of-fluid (VOF) method in the resolved macropores and tended towards the multiphase 122 Darcy model in the unresolved porous regions. Nonetheless, the gravity and capillary effects were not accounted for within the unresolved porous domain. Carrilo et al.<sup>16</sup> later proposed an improved 123 124 multiphase micro-continuum model with a theoretical derivation rooted in elementary physics and 125 volume-averaging principles. The critical feature of this improved multiphase micro-continuum 126 model is its rigorous derivation of multiscale parameters, including the relative velocity  $v_r$ , drag 127 force coefficient  $\mu k^{-1}$ , and capillary force  $F_c$ , which complement the sub-grid relative 128 permeability, gravity, and capillary effects. The physical meaning and mathematical formulation of these multiscale parameters differs in the resolved and unresolved porous media, allowing the 129 130 improved DBS multiphase model to asymptotically match the scale-dependent multiphase model, 131 i.e., the VOF model at the pore scale and the multiphase Darcy's law at the continuum scale. The 132 theoretically sound micro-continuum model was verified using numerical cases consisting of 133 continuum-scale, pore-scale, and hybrid-scale multiphase flows.<sup>16</sup>

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TABLE I. A summary of the development and application of the micro-continuum model.

Year	Authors	Equations	Fluid	Remarks	Reference
1949	Brinkman	Darcy- Brinkman (DB)	single phase	presented the DB equation for single-phase flow on a dense swarm of particles.	[30]

1967	Beavers et al.	Darcy- Brinkman (DB)	single phase	established Beavers-Joseph boundary conditions to simultaneously solve flow through porous and solid-free	[28]
1990	Hsu and Cheng	Darcy- Brinkman- Stokes (DBS)	single phase	regions. volume averaged the Navier- Stokes equations in a control volume containing fluids and solids.	[29]
2002	Golfier et al.	Stationary Darcy- Brinkman (DB)	single phase	simulated dissolution of porous media and characterized the influence of flow parameters on the wormhole development	[24]
2014	Horgue	Darcy- Brinkman- Stokes (DBS)	single phase	realized a complete workflow from pore-scale imaging to absolute permeability computation using the single- phase DBS model	[43]
2016	Soulaine et al.	Darcy- Brinkman- Stokes (DBS)	single phase	employed micro-continuum approach to model the flow, transport, and dissolution in fractured media	[15]
2018	Soulaine et al	Darcy- Brinkman- Stokes (DBS)	multiphase	proposed a micro-continuum approach to simulate the dissolution of minerals at the pore scale in the presence of multiple fluid phases	[18]
2020	Carrilo et al.	Darcy- Brinkman- Stokes (DBS)	single phase	derived, implemented, tested, and verified a multiscale model for two-phase flow in porous media.	[16]
2021	Xupeng He et al.	Darcy- Brinkman- Stokes (DBS)	single phase	simulated matrix-fracture interaction and fluid leakage using the single-phase DBS model.	[41]
2022	Hang Deng et al.	Darcy- Brinkman- Stokes (DBS)	single phase	performed simulations of dissolution-precipitation systems using the single- phase DBS model.	[42]
2022	Carrilo et al.	Darcy- Brinkman- Stokes (DBS)	multiphase	studied the influence of flow within the sub-resolution porosity on multiphase flow in heterogeneous porous media.	[39]

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137 Several limitations in the multiphase micro-continuum model persist. First, the application of 138 the current model is limited to multiphase drainage and imbibition with high capillary numbers of  $Ca = \mu u / \sigma = 10^{-1}$  to  $10^{-2}$ ,<sup>16</sup> where  $\mu$  is the characteristic dynamic viscosity, u is the inlet 139 140 velocity, and  $\sigma$  is the interfacial tension. In this situation, the viscous force dominates the 141 interfacial dynamics over the capillary force. However, for natural subsurface transport problems, the capillary forces are more significant, generally resulting in capillary numbers of 10<sup>-4</sup> or less.<sup>9,44</sup> 142 143 At low capillary numbers, spurious currents often appear near the gas-liquid interface and the three-144 phase contact-line region.<sup>45</sup> If the interface tension model is not handled carefully, these spurious currents could become larger than the physical flow, leading to unphysical fluid dynamics.<sup>9, 44</sup> 145 146 Therefore, the predictive capacity of the multiphase micro-continuum model in a multiscale porous 147 medium must be evaluated and improved at low capillary numbers. Second, similar to the top-down 148 definition of the contact angle in the classic VOF approach, the multiphase micro-continuum model 149 treats the contact angle  $\theta$  as an upscaled parameter, depending on the sub-grid-scale information.<sup>16</sup> 150 The current model inherits the correction strategy of the VOF approach to guarantee the interface on the porous boundary has a prescribed contact angle  $\theta$ .<sup>16, 18, 43</sup> Accordingly, the contact angle 151 correction is achieved by replacing the calculated normal to the gas-liquid interface  $n_{10}$  with the 152 locally modified norm  $\tilde{n}_{lg}$  to satisfy the wettability condition  $\tilde{n}_{lg} = \cos\theta n_p + \sin\theta t_p$ , where  $n_p$ 153

and  $t_p$  are the normal and tangent vectors to the porous boundary, respectively. As opposed to the standard boundary condition (a solid wall once rock-occupied cells have been removed from the mesh) in the VOF approach (see FIG. 1), liquid-statured or gas-saturated porous regions impact the saturation gradient  $\nabla \alpha_1$  at the porous boundary. This results in an unintended normal to the gas-

158 fluid interface of  $n_{lg} = \nabla \alpha_1 / \|\nabla \alpha_1\|$ . As such, the corrected contact angle arising from the abnormal

 $n_{lg}$  significantly deviates from the imposed contact angle in the capillary rise case studied by 159 Carrilo et al.<sup>16</sup> Third, the smoothed normal vector to the porous boundary  $n_{wall}$  is essential for 160 161 alleviating the spurious velocity near the contact-line region. In the classic VOF approach, an unstructured mesh is used to match the solid boundary and smooth the solid wall-normal vector.<sup>46,</sup> 162 <sup>47</sup> In contrast, the micro-continuum model uses structured Cartesian grids, with a staircase mesh 163 used to approximate the porous boundary.<sup>16, 31</sup> The resulting normal vector to the porous boundary 164  $n_{\rm p}$  does not provide smoothing, particularly at sharp corners. Therefore, the smoothing scheme of 165 166 the normal vector to the porous boundary should be investigated to achieve the stable simulation of





FIG. 1. Schematic representation of contact angle correction: (a) VOF approach, (b) multiphase micro-continuum approach. The red solid arrow represents the calculated normal to the gas-liquid interface  $n_{lg}$  and the purple dotted line represents the correct direction of  $n_{lg}$ .

168 This paper improves the multiphase micro-continuum DBS model to achieve stable 169 simulations of the two-phase flow at capillary numbers as small as 10<sup>-4</sup>. Particular attention is paid 170 to spurious velocities at the gas-liquid interface and contact-line region. First, we demonstrate how 171 different unit normal vectors to the gas-liquid interface impact the interface curvature and spurious 172 currents. Accordingly, a new formulation of the unit normal vector to the gas-liquid interface is 173 proposed. This formulation reduces the spurious velocities by at least one order of magnitude 174 compared with that of the interFoam model (the standard VOF-based solver in OpenFOAM). 175 Second, a saturation extrapolation algorithm is devised to reconstruct the saturation gradient near 176 the porous boundary, such that the correction strategy in the VOF approach can accurately enforce 177 the expected contact angle. Third, regarding the porous surface represented by a staircase 178 approximation, a weighted scheme for smoothing the normal to the porous boundary is developed 179 to eliminate the spurious currents near the contact-line region. Finally, the developed model is 180 verified by various test cases in which the results are compared with those obtained analytically or 181 from the *interFoam* solver. The test cases include a stationary gas bubble, droplets on flat and curved 182 surfaces, capillary rise, and liquid drainage in complex porous media.

183 The remainder of this paper is organized as follows. In Section II, mathematical models for the 184 multiphase micro-continuum DBS framework are introduced. Section III describes the improved 185 numerical models, equation discretization, and solver workflow based on the OpenFOAM open-186 source simulation platform. In Section IV, a series of validation cases for the multiphase flow are 187 presented. Finally, Section V summarizes the conclusions to this study.

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## 189 II. MATHEMATICAL MODELS

190 The two-phase micro-continuum framework consists of partial differential equations, which 191 are averaged over control volumes to govern the conservation of mass, momentum, and fluid 192 saturation, and can be solved for the single-field variables  $\bar{v}$ , p, and  $\alpha_1$ . In image-based 193 simulations, the control volumes correspond to the image voxels, which can contain one or two fluid 194 phases  $(V_1/V_g)$ , a solid phase  $(V_s)$ , or fluid/solid aggregates. Concerning the content within each 195 control volume, the averaged single-field variables are closely related to the local porosity field  $\varepsilon_f$ 196 and the saturation field  $\alpha_1$ , which are defined as

$$\varepsilon_{\rm f} = \frac{(V_{\rm l} + V_{\rm g})}{V},\tag{1}$$

$$\alpha_{\rm l} = \frac{V_{\rm l}}{V_{\rm l} + V_{\rm g}} \,. \tag{2}$$

197 The local porosity field is used to describe multiscale pore structure, consisting of resolved 198 macropores ( $\varepsilon = 1$ ), unresolved porous regions ( $0 < \varepsilon < 1$ ), and impermeable solid regions ( $\varepsilon \approx 0$ ). 199 The saturation field is defined as the ratio of the liquid volume over the total fluid phase volume 200 within each control volume. According to the local porosity field and the saturation field, the single-201 field variables are defined throughout the computational domain as

$$\overline{p} = \alpha_1 \overline{p}_1^1 + \alpha_g \overline{p}_g^g, \tag{3}$$

$$\overline{\mathbf{v}} = \varepsilon(\alpha_{\rm l} \overline{\mathbf{v}}_{\rm l}^{\rm l} + \alpha_{\rm g} \overline{\mathbf{v}}_{\rm g}^{\rm g}). \tag{4}$$

Here,  $\overline{p}$  is the averaged pressure over the control volume, while  $\overline{p}_i^i$  (i=l, g) denotes the averaged pressure over the phase. The same notation is applied to the velocity  $\boldsymbol{v}$ . Assuming the fluid phases to be incompressible, isothermal, and immiscible, the single-field continuity equation, saturation equation, and momentum equation in the multiphase micro-continuum DBS framework can be written as<sup>16</sup>

$$\nabla \cdot \overline{\mathbf{v}} = \mathbf{0},\tag{5}$$

$$\frac{\partial \varepsilon \alpha_{\rm l}}{\partial t} + \nabla \cdot \left(\alpha_{\rm l} \overline{\nu}\right) + \nabla \cdot \left(\varepsilon \alpha_{\rm l} \alpha_{\rm g} \overline{\nu}_{\rm r}\right) = 0, \tag{6}$$

$$\frac{1}{\varepsilon} \left( \frac{\partial \rho \overline{\boldsymbol{v}}}{\partial t} + \nabla \cdot \left( \frac{\rho}{\varepsilon} \overline{\boldsymbol{v}} \overline{\boldsymbol{v}} \right) \right) = -\nabla \overline{p} + \rho \mathbf{g} + \nabla \cdot \left( \mu \left( \nabla \overline{\boldsymbol{v}} + \nabla \overline{\boldsymbol{v}}^T \right) \right) - \mu k^{-1} \overline{\boldsymbol{v}} + \boldsymbol{F}_{c}.$$
(7)

In Eq. (7), the last term represents the surface tension forces, while the second-to-last term is the drag force, describing the porous resistance exerted on the pore walls. The governing equations above hold for the entire domain, regardless of the phases occupying the cells. In the resolved

macropore regions, the multiphase micro-continuum model matches the standard VOF-based Navier–Stokes equation, and so the saturation field delineates the liquid phase ( $\alpha_1 = 1$ ),gas phase ( $\alpha_1 = 0$ ), and the gas–liquid interface ( $0 < \alpha_1 < 0$ ). In contrast, the multiphase micro-continuum model tends asymptotically to the two-phase Darcy equation, in which the saturation field represents the actual liquid saturation. The scale-dependent behavior of the micro-continuum model is

215 achieved by a set of multiscale parameters  $\bar{v}_r, \rho, \mu k^{-1}$ , and  $F_c$ , which are derived through volume

- averaging and asymptotic matching principles.<sup>16</sup>
- 217 The relative velocity  $\overline{v}_r$  is given by<sup>16</sup>

$$\bar{\boldsymbol{v}}_{r} = \begin{cases} C_{\alpha} \max(|\bar{\boldsymbol{v}}|) \frac{\nabla \alpha_{1}}{|\nabla \alpha_{1}|}, & \text{in macropore regions} \\ -\left(\frac{M_{1}}{\alpha_{1}} - \frac{M_{g}}{\alpha_{g}}\right) \nabla \bar{p} + \left(\frac{\rho_{1}M_{1}}{\alpha_{1}} - \frac{\rho_{g}M_{g}}{\alpha_{g}}\right) \mathbf{g} \\ + \left(\frac{M_{1}\alpha_{g}}{\alpha_{1}} + \frac{M_{g}\alpha_{1}}{\alpha_{g}}\right) \nabla p_{c} - \left(\frac{M_{1}}{\alpha_{1}} - \frac{M_{g}}{\alpha_{g}}\right) p_{c} \nabla \alpha_{1} \end{cases}, & \text{in porous regions} \end{cases}$$
(8)

where  $C_{\alpha}$  is the interface compression coefficient, which is empirically determined as a value 218 between 0 and 4.  $M_i = \frac{k_0 k_{r,i}}{\mu_i}$  (i = l,g) is the mobility of fluid phase i, where  $k_0$  is the absolute 219 220 permeability of the porous medium and  $k_{r,i}$  is the relative permeability of fluid phase i. In the 221 macropore regions, the relative velocity is given by the classic VOF approach, which is active at the gas-liquid interface to sharpen the interface in the normal direction  $n_{lg} = \frac{\nabla \alpha_1}{|\nabla \alpha_1|}$  with an amplitude 222 223 based on the maximum single-field velocity. In the porous regions, the formulation of the relative 224 velocity can be derived by matching the formulation of the micro-continuum model to the two-225 phase Darcy model. Notably, the relative velocity in the porous regions is related to the phase 226 mobility  $M_i$ , gravitational acceleration g, and macroscopic capillary pressure  $p_c$ . As a result, the 227 relative velocity can account for the comprehensive interplay of the relative permeability, gravity, 228 and capillary effects. Conventionally, the relative permeability  $k_{r,i}$  and the macroscopic capillary 229 pressure  $p_c$  are represented as functions of saturation to complement the sub-grid hydrodynamic 230 impact of the porous micro-structure at the continuum scale. Relative permeability models, such as the Brooks and Corey model,<sup>20</sup> and capillary pressure models, such as the Van Genutchen model,<sup>19</sup> 231 232 are summarized in the literature.<sup>16</sup>

233 The formulation of the capillary force  $F_c$  significantly differs from the content of the grid 234 cell, as shown by Eq. (9). In the macropore regions, the capillary force emerges at the curved phase 235 interface to balance the pressure gradient. Here, the well-known continuum surface force (CSF) 236 formulation is adopted to quantify the capillary force.<sup>48</sup> The CSF model assumes the surface tension 237 to be constant within each control volume, and then approximates the volume-averaged surface

238 tension force in terms of the mean interface curvature. The mean interface curvature  $\bar{\kappa} = \nabla \cdot (n_{\rm lg})$ 

239 is estimated from the normal to the gas-liquid interface,  $n_{1s}$ . Note that some variants of the CSF

240 model, such as the sharp surface force (SSF) model, mitigate the magnitude of spurious currents at the gas-liquid interface.<sup>9, 46</sup> However, our numerical experiments found that, although the SSF 241 242 model can work well in some simple structures, such as stationary gas bubbles, alleviating the 243 spurious velocities becomes practically ineffective in complex porous media with significant 244 contact-line regions. For this reason, the SSF model is not applied in this work. Instead, numerical 245 approaches for the micro-continuum framework are introduced in Section III to effectively suppress 246 the spurious currents in the porous medium based on the CSF model. Similar to the relative velocity 247  $\overline{v}_r$ , the capillary force in the porous regions can be determined from the two-phase Darcy model.

$$F_{\rm c} = \begin{cases} -\varepsilon^{-1}\sigma \nabla \cdot (\boldsymbol{n}_{\rm lg}) \nabla \alpha_{\rm l}, & \text{in macropore regions} \\ \\ \begin{bmatrix} M^{-1} (M_{\rm l}\alpha_{\rm g} - M_{\rm g}\alpha_{\rm l}) (\frac{\partial p_{\rm c}}{\partial \alpha_{\rm l}}) - p_{\rm c} \end{bmatrix} \nabla \alpha_{\rm l}, & \text{in porous regions} \end{cases}$$
(9)

248 The drag force coefficient quantifies the relation between the fluid-solid friction and the single-249 field velocity. In the porous regions, the drag force coefficient is defined by a harmonic average of 250 the gas and liquid phase mobility, as given by Eq. (10); in the macropore regions, it vanishes to zero. 251 Unlike the artificial modification of the drag force term with respect to the solid content in grid cells, 252 the dissipative viscous term is retained in the DBS momentum model. However, the relative 253 magnitude between the porous drag force term and the dissipative viscous term naturally varies 254 from the make-up of the grid cells. The porous drag force term gradually becomes dominant over the dissipative viscous term with  $0 < \varepsilon < 1$ .<sup>15,49</sup> This gradual transition ensures the continuity of the 255 stress and velocity in the entire computational domain.<sup>22</sup> Eventually, together with the scale-256 257 separated definition of the capillary force in Eq. (9) and the fluid density in Eq. (11), the micro-258 continuum model reduces to the two-phase Darcy solution for the description of the continuum-259 scale multiphase flow in the porous regions and to the VOF approach for explicitly tracking the gas-260 liquid interface and three-phase contact lines in the macropore regions.<sup>16</sup>

$$\mu k^{-1} = \begin{cases} 0, & \text{in macropore regions} \\ k_0^{-1} \left( \frac{k_{r,1}}{\mu_1} + \frac{k_{r,g}}{\mu_g} \right)^{-1}, & \text{in porous regions} \end{cases}$$
(10)

$$\rho = \begin{cases}
\rho_1 \alpha_1 + \rho_g \alpha_g, & \text{in macropore regions} \\
\left(\rho_1 M_1 + \rho_g M_g\right) M^{-1}, & \text{in porous regions}
\end{cases}$$
(11)

261 Similar to the solid wall, the porous boundary between the macropore and porous regions 262 produces wall adhesion forces due to uneven molecular forces along the contact lines. Theoretically, the macroscopic contact angle at the porous boundary is related to various sub-grid interface properties, such as the fluid interfacial tension, porous microstructure, and spreading film shape.<sup>50</sup> However, this study treats the contact angle as an upscaled parameter and only considers the macroscopic contact-line dynamics. Therefore, the normal to the gas–liquid interface at the porous boundary is modified according to Eq. (12) to ensure that the contact angle is equal to the prescribed value of  $\theta$ :

$$\tilde{n}_{\rm lg} = \cos\theta n_{\rm p} + \sin\theta t_{\rm p},\tag{12}$$

269 where  $n_{\rm p}$  and  $t_{\rm p}$  are the normal and tangent vectors to the porous boundary, respectively.

- According to Horgue et al.<sup>43</sup> and Soulaine et al.,<sup>18</sup> Eq. (12) can be recast into the formulation of Eq.
- 271 (13) for convenient computation:

$$\tilde{\boldsymbol{n}}_{lg} = \frac{\cos\theta - \cos\theta_{l}\cos(\theta_{l} - \theta)}{1 - \cos^{2}\theta_{l}}\boldsymbol{n}_{p} + \frac{\cos(\theta_{l} - \theta) - \cos\theta_{l}\cos\theta}{1 - \cos^{2}\theta_{l}}\boldsymbol{n}_{lg},$$
(13)

where  $\theta_{I} = \cos^{-1}(n_{p} \cdot n_{lg})$  and  $n_{lg}$  is the normal to the gas-liquid interface yielded by the current saturation field. These values may not satisfy the targeted wettability condition and should be corrected to  $\theta$  and  $\tilde{n}_{lg}$ , respectively.

In conclusion, Eq. (7) constitute the governing equations, and Eq. (9) closure the equations by defining the relative velocity  $\bar{v}_r$ , the drag force  $\mu k^{-1}$ , and the surface tension force  $F_c$ , in both macropore and porous regions . Eq. (13) is used to correct the calculated contact angle to the prescribed value.

279

280 III. NUMERICAL METHODS

281 The finite volume method (FVM) is used to solve the mathematical model, where the partial 282 differential equations are first discretized by integrating them over each control volume to yield a 283 set of algebraic equations. To achieve an acceptable magnitude for the spurious velocities at 284 capillary numbers as low as 10<sup>-4</sup>, particular attention is paid to the discretization of the capillary 285 force at the gas-liquid interface and the contact-line region. A hybrid formulation of the unit normal 286 vector to the gas-liquid interface is proposed to enable accurate computations of the interface 287 curvature. Concerning the multiscale nature of the micro-continuum framework, the saturation 288 extrapolation algorithm is introduced to correct the normal to the gas-liquid interface at the porous 289 boundary. Combined with an improved smoothing scheme of the normal to the staircase-like porous 290 interface, the prescribed contact angle and the reduced spurious velocity can be achieved at the 291 contact-line region. Finally, essential information on the equation discretization and solver

workflow is introduced.

# 293

## **A.** Discretization of the normal to the gas–liquid interface

295 In the macropore regions, the multiphase micro-continuum DBS model reduces to the classic 296 VOF-based Navier-Stokes equation, where the capillary force is described as a body force by the 297 CSF model in Eq. (9). The inaccurate estimation of the interface curvature in the CSF model is 298 believed to destroy the balance of the interfacial forces and intensify the non-physical spurious currents.9, 44 According to the volume-averaging derivation, the interface curvature within the 299 control volume is approximated as the mean curvature, which can be obtained by  $\bar{\kappa} = -\nabla \cdot \boldsymbol{n}_{i_{\alpha}}$ . 300 301 Numerically, the semi-discretized form of the interface curvature can be obtained using the Gaussian 302 scheme

$$\overline{\kappa} = -\sum_{V_i} \frac{1}{V_i} n_{\lg, f} \cdot S_f \,, \tag{14}$$

303 where the subscript *f* denotes the field on face *f* of the control volume,  $S_f$  is the outward pointing 304 face surface vector, and  $V_i$  is the volume of grid cell i. In the *interFoam* (the VOF-based solver in 305 OpenFOAM) and *hybridPorousInterFoam* (open-source implementation of the multiphase micro-306 continuum model developed by Carrillo et al.<sup>51</sup>) solvers, the face-centered interface norm  $n_{lg,f}$  is

307 calculated by the face-centered saturation gradient divided by its magnitude, i.e.,

$$\boldsymbol{n}_{\mathrm{lg},f} = \frac{\left\langle \nabla \alpha_{\mathrm{l}} \right\rangle_{c \to f}}{\left\| \left\langle \nabla \alpha_{\mathrm{l}} \right\rangle_{c \to f} \right\|},\tag{15}$$

308 where  $\langle \rangle_{c \to f}$  denotes the interpolation operator from the cell-centered field to the face-centered 309 field. This formulation is based on the interpolated saturation gradient, and is referred to hereafter 310 as the IG scheme. In contrast to the IG scheme, the *poreFoam* (open-source two-phase flow solver 311 developed by Raeini et al.<sup>9</sup> and Shams et al.<sup>44</sup>) and *interGCFoam* (open-source multiphase flow and 312 transport solver developed by Maes et al.<sup>52</sup>) methods adopt a different formulation, referred to 313 hereafter as the IN scheme, which directly interpolates the cell-centered unit normal to the face-314 centered unit norm as

$$\boldsymbol{n}_{\rm lg} = \frac{\nabla \alpha}{\|\nabla \alpha\|}, \ \boldsymbol{n}_{\rm lg,f} = \left\langle \boldsymbol{n}_{\rm lg} \right\rangle_{c \to f}.$$
(16)

The IG and IN schemes underestimate and overpredict, respectively, the interface curvature in numerical experiments. As illustrated in FIG. 2(a), the underlying reason for the underestimation of curvature by the IG scheme is that the interpolated saturation gradient at the face center favors neighboring cell-centered saturation gradients with larger magnitudes, leading to the interpolated

319 saturation gradient around the grid cell faces being somewhat similar. According to Eq. (14), the 320 numerical surface integral of unit vectors of these interpolated saturation gradients on the cell faces 321 offsets some of the flux fields from the similar components, resulting in an underestimated curvature. 322 By comparison, the IN scheme in FIG. 2(b) adopts the unit normal to the gas-liquid interface with 323 a magnitude of one to ensure the independent contribution of the neighboring cell-centered unit 324 norms to the interpolated face-centered unit norm. Therefore, the IN scheme does not underestimate 325 the curvature. Nonetheless, some curvature overprediction is produced by the IN scheme. This is 326 thought to come from the inherent error of the numerical method, which uses the mean curvature to 327 represent the local curvature at every point of the gas-liquid interface within the grid cell. In the 328 low-capillary-number regime, where the capillary force becomes dominant, the discrepancies in the 329 interface curvature given by both the IG and IN schemes becomes non-negligible and produces 330 significant spurious velocities at the phase interface.



FIG. 2. Graphic representation of cell-centered or face-centered vectors for computing the normal to the gas-liquid interface. (a) Saturation gradients in the IG scheme, (b) normal to the gas-liquid interface in the IN scheme. The black solid arrows represent the cell-centered vectors, while the red dashed arrows depict the face-centered vectors. The gray dashed arrows are formed by moving the cell-centered vectors parallel to the face center for comparison.

331

For a more accurate computation of the face-centered normal to the gas-liquid interface, a 332 hybrid formulation is proposed in which the counter-impacts of the IG and IN schemes on the 333 interface curvature are neutralized:

$$\boldsymbol{n}_{\mathrm{lg},f} = C_{\mathrm{lg}} \left\langle \frac{\nabla \alpha}{\|\nabla \alpha\|} \right\rangle_{c \to f} + \left(1 - C_{\mathrm{lg}}\right) \frac{\langle \nabla \alpha_1 \rangle_{c \to f}}{\left\| \langle \nabla \alpha_1 \rangle_{c \to f} \right\|}.$$
(17)

334 A value of  $C_{lg} = 0$  reduces to the IG scheme, while as  $C_{lg}$  approaches 1, the hybrid formulation

reduces to the IN scheme. Because the underprediction by the IG scheme is more serious than the

336 overestimation by the IN scheme, a value of  $C_{lg} = 0.6$  is used in the following simulations.

337

## **B.** Correction of the normal to the gas–liquid interface at the porous boundary

339 After solving the saturation fields, the obtained normal vector to the gas-liquid interface  $n_{l_{10}}$ 340 is used to correct the contact angle at the porous boundary according to Eq. (13). In the micro-341 continuum framework, the correction strategy for the contact angle is taken from the classic VOF 342 approach.<sup>14, 43</sup> However, different representations of porous media change the direction of the 343 normal vector to the gas-liquid interface at the solid/porous boundary, as shown in FIG. 3. In FIG. 344 3(a), the VOF approach removes the solid phase from the mesh, and the solid surface is treated as 345 the conventional wall boundary. Accordingly, the normal to the gas-liquid interface is calculated 346 based on the known saturation field within the bulk fluid phase. In contrast, all the grid cells are 347 retained in the micro-continuum framework to describe the multiscale porous medium. They must 348 have nonzero porosity, suggesting that a low-porosity, low-permeability domain will have little void 349 space occupied by the gas or liquid phase. As shown in FIG. 3(b), highly contrasting saturation 350 fields may exist in the solid-free and porous regions, both of which participate in computing the 351 normal to the gas-fluid phase at the porous boundary. As such, the obtained interface norm deviates 352 from its original definition for the contact angle correction algorithm. Furthermore, the nonzero 353 saturation gradient at these porous boundaries introduces a non-physical capillary force and spurious 354 currents. To deal with this problem, the saturation of the solid-free region is extrapolated to the 355 nearby porous region according to Eqs. (18) and (19). As illustrated in FIG. 3(c), the neighboring 356 saturation field at either side of the porous boundary becomes the same to eliminate the component 357 of the saturation gradient pointing from the porous region to the solid-free region. Therefore, the 358 saturation extrapolation algorithm recovers the magnitude and direction of the saturation gradients 359 at the contact-line region to be consistent with the VOF approach. Moreover, the saturation gradient 360 that should not exist along the porous boundary vanishes.

(a)				(b)					(c)									
1	1	1	Y	4	0	1	1	1	Y	<b>~</b> 0	0		1	1	1	Y	4	0
1	1	$\mathbf{Y}$	ኤ	0	0	1	1	'ı	×o	0	0		1	1	Ì	≻₀	0	0
1	-1	$\sim$	0	0	0	1	-1	<u>_</u> 0	ę	ę	ę		1	⊷1	X	0	0	0
						1	1	1	1	1	1		1	1	0	0	0	0
						1	1	1	1	1	1		1	1	1	1	1	1

FIG. 3. Graphic representation of the normal to the gas–liquid interface close to the solid/porous boundary: (a) VOF approach, (b) non-corrected normal vectors in the multiphase multiscale model, (c) illustration of the saturation extrapolation from the solid-free region to the porous region and the corrected normal vectors in the multiphase multiscale model. White cells represent the solid-free region, gray cells indicate the porous region, and arrows depict the normal vector to the gas–liquid interface.

$$\chi = \begin{cases} 1, \text{ in the macropore region} \\ 0, \text{ in the porous region} \end{cases}, \quad \chi_f = \operatorname{ceil}(\langle \chi \rangle_{c \to f}), \tag{18}$$

$$\alpha_{l,corr} = \begin{cases} \chi \alpha_{l} + (1-\chi) \frac{\left\langle \chi_{f} \left\langle \alpha_{l} \right\rangle_{c \to f, harmonic} \right\rangle_{f \to c}}{\left\langle \chi_{f} \right\rangle_{f \to c}}, & \alpha_{l,solid} = 1 \\ 1 - \left( \chi (1-\alpha_{l}) + (1-\chi) \frac{\left\langle \chi_{f} \left\langle 1-\alpha_{l} \right\rangle_{c \to f, harmonic} \right\rangle_{f \to c}}{\left\langle \chi_{f} \right\rangle_{f \to c}} \right), & \alpha_{l,solid} = 0 \end{cases}$$

$$(19)$$

361 where  $\chi$  is an indicator function representing whether the grid block belongs to the resolved 362 macropore region or the unresolved porous region. The computation of  $\alpha_{l,corr}$  depends on the 363 occupied phase in the void space of the porous regions, as given by Eq. (19), where  $\langle \rangle_{f \to c}$ 

represents interpolation from face center to cell center, while  $\langle \rangle_{c \to f}$  represents interpolation from cell center to face center. The subscript "harmonic" denotes the harmonic-mean scheme used in the interpolation.

367

## 368 C. Smoothing of the normal to the porous boundary

The normal to the porous boundary is another critical input for the contact angle correction in the contact-line region, as shown by Eq. (13). Concerning the structured Cartesian grid used in the multiphase micro-continuum approach, the normal vectors should be smoothed to represent the complex porous boundaries, which is effective for reducing spurious velocities and improving numerical stability. The *hybridPorousInterFoam* code<sup>16</sup> adopts Eqs. (20)–(24) to smooth the normal to the fluid–solid interface:

$$\boldsymbol{n}_{\mathrm{p},f} = \frac{\nabla \varepsilon_f}{\left\|\nabla \varepsilon_f\right\|},\tag{20}$$

$$\xi_f = \left\| \boldsymbol{n}_{\mathrm{p},f} \right\|,\tag{21}$$

$$\nabla \varepsilon_{f,i} = \xi_f \left\langle \left\langle \nabla \varepsilon_{f,i-1} \right\rangle_{f \to c} \right\rangle_{c \to f}, i = 1 \sim n - 1,$$
(22)

$$\nabla \varepsilon_{f,n} = \left\langle \left\langle \nabla \varepsilon_{f,n-1} \right\rangle_{f \to c} \right\rangle_{c \to f},\tag{23}$$

$$\tilde{\boldsymbol{n}}_{p,f} = \frac{\nabla \boldsymbol{\varepsilon}_{f,n}}{\left\| \nabla \boldsymbol{\varepsilon}_{f,n} \right\|},\tag{24}$$

where  $\nabla_{\mathcal{E}_f}$  is the face-centered gradient of the local porosity  $\varepsilon$ ,  $\xi_f$  is an indicator function 375 representing the porous boundary, and  $n_{p,f}$ ,  $\tilde{n}_{p,f}$  are the raw and smoothed unit norms to the 376 377 porous surface, respectively. The key steps are implemented by Eqs. (22) and (23), which interpolate 378 the gradient of the local porosity from face centers to cell centers and then back to the face centers recursively for i iterations (i≥1). Concerning the smoothing kernel  $\langle \langle \rangle_{f \to c} \rangle_{c \to f}$ , which diffuses the 379 380 smoothed variable away from the porous boundary, the coefficient  $\xi_f$  is applied before the kernel 381 in Eq. (22) to limit  $\nabla \varepsilon_{f,i}$  on the porous boundary. Such smoothed normalized norms to the porous 382 boundaries  $\tilde{n}_{p,f}$  are illustrated in FIG. 4. The smoothed norms still spread into the vicinity close 383 to the porous boundary due to the absence of a location constraint in Eq. (23). The diffused norms 384 to the porous boundaries  $\tilde{n}_{p,f}$  induce the unexpected correction of the normal to the gas-liquid interface  $\tilde{n}_{lg}$  in the vicinity of the porous surface through Eq. (13) and then produce an ill-balanced 385 386 capillary force in Eq. (9). Finally, spurious velocities are intensified by these smoothed norms to the 387 porous boundary in the contact-line region.



FIG. 4. Schematic illustration of normal vectors to the porous boundary: (a) example 1 with a curved porous boundary, (b) example 2 with a sloped boundary. The blue arrows represent the smoothed normal vectors given by the *hybridPorousInterFoam* solver, while the red arrows depict the smoothed normal vectors produced by the proposed method. The black lines delineate the curved or sloped porous boundary ( $\varepsilon = 0.5$  iso-surface).

388 To model the normal to the porous boundary accurately, a weighted smoothing method is 389 proposed in Eqs. (27) and (28). The previous and present norms to the porous boundaries are 390 compared in FIG. 4, which shows that the present smoothed norms are successfully limited on the 391 porous boundaries. Moreover, a visual inspection finds that the present smoothed normal vectors 392 are more perpendicular to the curved and sloped porous boundaries than the previous smoothed 393 normal vectors. The improved orthogonal property of the present smoothed norms can be attributed 394 to the change in the smoothed vector from the gradient of the local porosity in Eqs. (22) and (23) to 395 the unit normal to the porous boundary in Eqs. (27) and (28). Similar to the difference between the 396 IG and IN schemes for computing the normal to the gas-liquid interface, as discussed in Section 397 III.A, the adoption of the non-normalized gradient in Eqs. (22) and (23) distorts the direction of the 398 normal to the porous boundary, which moves toward the neighboring gradient with a larger 399 magnitude.

$$\boldsymbol{n}_{\mathrm{p}} = \frac{\nabla \varepsilon}{\left\| \nabla \varepsilon \right\|} \tag{25}$$

$$\xi = \left\| \boldsymbol{n}_{\mathrm{p}} \right\| \tag{26}$$

$$\tilde{\boldsymbol{n}}_{p}^{*} = \xi \left\langle \left\langle \xi \boldsymbol{n}_{p} \right\rangle_{c \to f} \right\rangle_{f \to c} / \left\langle \left\langle \xi \right\rangle_{c \to f} \right\rangle_{f \to c}$$

$$\tag{27}$$

$$\tilde{\boldsymbol{n}}_{\mathrm{p},f} = \left\langle \frac{\tilde{\boldsymbol{n}}_{\mathrm{p}}^{*}}{\left\| \tilde{\boldsymbol{n}}_{\mathrm{p}}^{*} \right\|} \right\rangle_{c \to f}$$
(28)

400

#### 401 **D.** Equation discretization

402 The solver is developed based on the open-source *hybridPorousInterFoam* solver,<sup>16</sup> which is 403 the first implementation of the multiphase micro-continuum model with the FVM based on OpenFOAM.<sup>51, 53, 54</sup> The open-source code can be accessed from the author's repository 404 405 (https://github.com/anoldfriend0718/multiscalePorousFoam). We welcome the interested reader to 406 review the numerical code, reproduce simulation cases and contribute to further model development. 407 In the FVM, the governing equations are first discretized by integrating over each control volume 408 at the given time step to yield a set of algebraic equations. The pressure equation should be 409 formulated by combining the semi-discretized gas continuity and DBS momentum equations to 410 account for the velocity-pressure coupling. A detailed derivation of the semi-discretized pressure equation can be found in the literature.<sup>16, 31</sup> The first-order *Euler* time scheme is used to discretize 411 412 the time derivative  $\partial/\partial t$  terms, while the spatial terms are discretized using second-order numerical 413 schemes. The gradient term  $\nabla$  is discretized by the *Gauss linear* scheme, with a linear scheme 414 implemented for the value interpolation from cell centers to face centers. The Gauss vanLeerV

415 scheme is employed for the divergence term  $\nabla \cdot (\frac{\rho}{\varepsilon} \overline{v} \overline{v})$ , while the *Gauss vanLeer* scheme is 416 performed for  $\nabla \cdot (\alpha_1 \overline{v})$ . For the compression term in the saturation equation, the interpolation of 417  $\alpha_1 \alpha_g$  is implemented using the *interfaceCompression* scheme. The Laplacian term for the 418 dissipative viscous force  $\nabla \cdot (\mu (\nabla \overline{v} + \nabla \overline{v}^T))$  is calculated using the Gauss linear corrected scheme. 419 420 **E.** Numerical workflow

421 Sequential coupling strategies are introduced to solve the discretized governing equations for 422 the nonlinear problem, as illustrated in FIG. 5. In the numerical workflow, the pressure–velocity 423 coupling is handled using the pressure implicit with splitting of operators (PISO) algorithm<sup>55</sup> to 424 solve the DBS momentum equations. The constraint on the time step is imposed by the Brackbill 425 condition<sup>48</sup> to ensure numerical stability through the explicit treatment of the surface tension force:

$$\Delta t < \sqrt{\frac{\rho_{\text{ave}} \left(\Delta x\right)^3}{2\pi\sigma}},\tag{29}$$

426 where  $\rho_{ave}$  is the average phase density and  $\Delta x$  is the grid spacing. The main iterative procedure 427 in advancing the time step from n to n+1 is described as follows.

- 428 (1) Solve the saturation equation (6) using the multidimensional universal limiter with explicit
   429 solution (MULES) algorithm<sup>56</sup> to ensure the saturation boundedness;
- 430 (2) Update fluid properties such as the density  $\rho^*$  and viscosity  $\mu^*$  and porous transport 431 properties such as the relative permeability  $\mu^*$ , phase mobility  $M_i^*$ , and capillary pressure  $p_c^*$ 432 based on the saturation field from the previous iteration;
- 433 (3) Extrapolate the saturation  $\alpha_{l,corr}^*$  from the solid-free region to the nearby porous region 434 according to Eq. (19) to correct the saturation gradient at the porous boundary;

435 (4) Calculate the normal to the gas-liquid interface  $n_{lg,f}^*$  via the hybrid formulation of Eq. (17);

- 436 (5) Compute and smooth the normal to the porous boundary  $\tilde{n}_{p,f}^*$  using Eqs. (27) and (28), and
- 437 then correct the normal to the gas–liquid interface  $\tilde{n}_{\lg,f}^*$  in the contact line regions according
- 438 to Eq. (13);
- 439 (6) Compute the interface curvature  $\bar{\kappa}^*$  from Eq. (14), and then update the surface tension force 440  $F_c^*$  using Eq. (9);



FIG. 5. Flowchart of the improved multiphase micro-continuum model.

- 441 (7) Solve the discretized DBS momentum equation (7) implicitly to predict the velocity  $\bar{v}^*$  and 442 the mass flux phi<sup>\*</sup>. Note that the predicted fields  $\bar{v}^*$  and phi<sup>\*</sup> do not satisfy the mass 443 conservation requirement after this prediction step;
- 444 (8) Solve the pressure equation implicitly with the preconditioned conjugate gradient method to
- 445 correct the pressure  $\overline{p}^{**}$  and update the velocity  $\overline{v}^{**}$  and mass flux phi<sup>\*\*</sup>. This step, called 446 the PISO loop, is repeated three times to ensure the pressure and velocity converge and satisfy 447 the mass conservation requirement.

#### 448

## 449 IV. VALIDATION CASES

450 A series of capillary-dominated two-phase flow tests are performed to verify that the improved 451 micro-continuum DBS model reduces the spurious velocities. Different interpolation schemes from 452 the interface normal to the gas-liquid interface are compared by simulating a stationary gas bubble 453 in liquid (Section IV.A). Droplets on flat and curved surfaces with hydrophilic, neutral, and 454 hydrophobic wettability boundary conditions are simulated to demonstrate the importance of the 455 correction scheme of the norms to the gas-liquid interface and the weighted scheme to the porous 456 boundary, respectively (Section IV.B). In terms of the multiphase flow dynamics in simple and 457 complex geometries, the improved DBS model is further verified by modeling capillary rise in a 458 single tube (Section IV.C) and liquid drainage in porous media (Section IV.D). The boundary 459 conditions and solver parameters are defined in FIG S1-S4 and TABLE S1-S4 in the Supplementary 460 Materials.

461

## 462 A. Stationary gas bubble

463 As a common test of two-phase flow models, simulating a gas-liquid system under equilibrium 464 conditions enables a simple examination of the spurious velocities induced due to ill-balanced 465 interface tension by measuring the maximum velocity in the computational domain. In this study, a 466 stationary gas bubble in liquid is simulated without gravity to compare the spurious velocities 467 produced by different interpolation schemes of the normal to the gas-liquid interface, including the 468 IG, IN, and hybrid schemes. As shown in FIG. 6(a), the gas bubble of diameter 2R is located at the 469 center of a square domain of length 4R, R is 10  $\mu$ m. Periodic boundary conditions are imposed on 470 all boundaries for pressure, velocity, and liquid saturation. The fluid densities and viscosities are  $\rho_1 = 1000 \text{ kg/m}^3 \text{ and } \rho_g = 1 \text{ kg/m}^3, v_1 = 10^{-6} \text{ m}^2/\text{s and } v_g = 1.48 \times 10^{-5} \text{ m}^2/\text{s}.$  The surface tension 471 472 is  $\sigma = 0.03$  kg/s<sup>2</sup>. The impact of the mesh resolution on the spurious velocity around the stationary 473 bubble is also investigated. TABLE II lists computational domain meshes with different 474 resolutions of  $R/\delta x$ , where  $\delta x$  is the length of the grid cell.

475

476 TABLE II. Details of mesh and maximum time step used for the stationary gas bubble simulations.

Mesh	Mesh resolution $(\mu m^2)$	Number of cells	$R/\delta x$	Maximum time step (s)
M1	0.625×0.625	64×64	16	2.3×10 <sup>-8</sup>
M2	0.5×0.5	80×80	20	1.6×10 <sup>-8</sup>
M3	0.4×0.4	100×100	25	1.2×10 <sup>-8</sup>

477

7 FIG. 6 compares the liquid saturation and surface tension force fields calculated using the IG,

478 IN, and hybrid schemes. In the magnified views of the gas-liquid interface shown in FIG. 6(b)-6(d),

479 the white lines represent the simulated gas-liquid interface and the black lines delineate the 480 theoretical gas-liquid interface. Although the simulated gas-liquid interfaces are generally rounded, 481 some deformations appear in the direction at an azimuth angle of around  $45^{\circ}$ , referred to as the  $45^{\circ}$ 482 direction, when using the IG and IN schemes. Compared with the theoretical gas-liquid interface, 483 the IG scheme raises the gas-liquid interface outwards, while the IN scheme collapses the gas-484 liquid interface inwards. The interface deformation in the 45° direction is related to the uneven 485 surface tension forces along the circumference, as depicted in FIG. 6(e) and 6(f) for the IG and IN 486 schemes, respectively. As discussed in Section III.A, the IG scheme underestimates the interface 487 curvature during the numerical surface integration based on the interpolated saturation gradient. The 488 underestimation becomes significant in the 45° direction. Consequently, the underestimated 489 interface curvature reduces the surface tension force and eventually produces a convex gas-liquid 490 interface. Conversely, the overpredicted interface curvature and surface tension given by the IN 491 scheme leads to a sunken gas-liquid interface. Considering the counter-impacts of the IG and IN 492 schemes, the hybrid scheme is intended to correct the numerical error of the interface curvature. As 493 shown in FIG. 6(g), a relatively uniform distribution of surface tension forces can be obtained from 494 the hybrid scheme, resulting in the closest solution to the theoretical gas-liquid interface in FIG. 495 6(d).



FIG. 6. Variations of simulated gas–liquid interfaces and surface tension forces under different interpolation schemes for the normal to the gas–liquid interface using the mesh resolution of  $R/\delta x=25$ : (a) overview of saturation field using the hybrid scheme; (b)–(d) magnified views of the gas–liquid interface using IG, IN, and hybrid schemes. The white lines represent the simulated gas–liquid interface, black lines represent the theoretical gas–liquid interface, and black arrows

represent the deformation direction; (e)–(g) magnified views of surface tension forces using IG, IN, and hybrid schemes, where gray arrows represent the surface tension force.

Besides interface deformation, the uneven surface tension force can induce spurious velocities.
 FIG. 7 compares the spurious capillary number using different mesh resolutions and interpolation

498 schemes. The magnitude of the spurious velocity is defined as

$$v_{\rm sp} = \max(|\overline{\boldsymbol{\nu}}|) \tag{30}$$

499 and the spurious capillary number is defined as

$$Ca_{sp} = \frac{\mu_l v_{sp}}{\sigma} \,. \tag{31}$$

500 FIG. 7(a) indicates that the spurious capillary number computed using the IG scheme ranges 501 from 10<sup>-3</sup> to 10<sup>-2</sup>, representing the largest magnitude and fluctuation among the three interpolation 502 schemes. For the IN scheme [FIG. 7(b)], the spurious capillary number is lower than in the IG 503 scheme, dropping to 10<sup>-5</sup>-10<sup>-3</sup>. In both the IG and IN schemes, the spurious capillary number 504 increases with the mesh resolution, that is, finer grid cells. Other researchers have also reported this 505 abnormal variation of spurious velocities with mesh resolution when using the conventional VOF model with the IG or IN scheme.44,57 One possible reason is that the curvature computation with a 506 507 finer mesh is more sensitive to numerical errors in the normal vector to the gas-liquid interface than 508 a coarse mesh. By comparison, FIG. 7(c) shows that the spurious capillary number using the hybrid 509 scheme converges to about 10<sup>-5</sup>, regardless of the mesh resolution, even though the finer mesh yields 510 more rapid convergence. This implies that the hybrid scheme is the most robust solution for 511 achieving low spurious velocities with various mesh sizes.



FIG. 7. Spurious capillary number based on the spurious velocities versus time using different mesh resolutions and interpolation schemes: (a) IG, (b) IN, (c) hybrid.

512 These results show that the IG and IN schemes cause interface deformations in opposite 513 direction due to the underestimated and overestimated surface tension forces. The proposed hybrid 514 scheme produces more accurate curvature values, effectively mitigating the interface deformation 515 and robustly reducing the spurious velocity to spurious capillary numbers of less than 10<sup>-5</sup> under

516 various mesh resolutions. What should be emphasized is that the hybrid scheme for the normal to 517 the gas-liquid interface is implemented based on the CSF model rather than the SSF model or its 518 variations. Even though the SSF model can reduce the spurious capillary number of static gas bubbles to the level of machine precision  $(10^{-15})$ ,<sup>9</sup> spurious currents still emerge when simulating 519 520 the multiphase flow dynamics in capillary-dominated regimes with Ca≤10<sup>-4</sup>. Section IV.D will show 521 that spurious currents of acceptable magnitude can also be achieved by the hybrid scheme based on 522 the CSF model with  $Ca=10^{-4}$ . In addition, considerable modifications must be applied to the 523 interface dynamics in the SSF model,<sup>52</sup> including smoothed saturation by a Laplacian smoother for 524 the calculation of interface curvature and sharpened saturation by a curtailment function for the 525 computation of the surface tension force.<sup>9</sup> For these reasons, the combination of the hybrid scheme 526 and the CSF model is used in the present study to ensure the numerical model is simple, physical, 527 and effective.

528

# 529 B. Stationary droplets on flat and curved surfaces

530 Using a classic test of stationary droplets on flat surfaces, the effect of the norm correction to 531 the gas-liquid interface at the porous boundary on the contact-line dynamics is investigated to verify 532 the improved DBS model. Particular attention is given to the contact angle and the spurious velocity 533 in the contact-line region at the equilibrium state. A semicircle droplet with a radius of 0.7 mm is 534 initialized on a flat surface, and three different contact angles of  $\theta = 60^\circ, 90^\circ, 135^\circ$  are prescribed. 535 In the micro-continuum DBS model, a porous plate with negligible porosity and permeability  $(\varepsilon = 0.01, k_0 = 10^{-16} \text{m}^{-2})$  is introduced to approximate the nonslip wall boundary based on a 536 penalization strategy.<sup>15</sup> To highlight the necessity of the saturation extrapolation algorithm during 537 538 the norm correction, a contrasting saturation is set up on the sides of the porous boundary, where 539 the porous substrate is saturated with the liquid, while the gas fills the upper clear fluid region except 540 for the liquid droplet. The fluid densities and viscosities in each phase are set as  $\rho_1 = 1000 \text{ kg/m}^3$ and  $\rho_g = 1 \text{ kg/m}^3$ ,  $v_1 = 10^{-6} \text{ m}^2/\text{s}$  and  $v_g = 1.48 \times 10^{-5} \text{ m}^2/\text{s}$ , respectively. The surface tension is 541 542  $\sigma = 0.03$  kg/s<sup>2</sup>. The computation is configured with a cell size of 12.5 µm and a time step of 0.5 543 μs.



FIG. 8. Liquid saturation fields of droplets on flat surfaces with different prescribed contact angles using: (a) original DBS and (b) improved DBS with saturation gradient correction. The solid white lines represent the gas–liquid interface ( $\alpha_1 = 0.5$  iso-surface), the solid black lines represent the fluid–solid interface ( $\varepsilon = 0.5$  iso-surface), black arrows represent the saturation gradient, and gray diagonals represent the porous region.

544 FIG. 8 compares the equilibrium saturation configurations of these droplets on flat surfaces 545 with three contact angles, each computed using the micro-continuum DBS model with and without 546 correcting the normal to the gas-liquid interface. In the magnified views of the contact-line region, 547 the simulated gas-liquid interface is delineated by the white line, and the saturation gradient is 548 represented by black arrows to visualize the cause of the numerical error in the contact angle. As 549 observed in FIG. 8(a) for the original DBS results, the contrasting saturation introduces nonzero 550 saturation gradients at the porous boundary, which should be zero in the conventional VOF approach 551 using the standard wall boundary rather than the porous plate. The resulting normal vector to the gas-liquid interface  $n_{lg}$  deviates from its original definition in the contact angle correction 552 553 algorithm of Eq. (13). The numerical error then propagates from the normal vector to the gas-liquid 554 interface  $n_{lg}$  into the capillary force  $F_c$  based on Eq. (9). Consequently, FIG. 9(a) clearly 555 illustrates that significant spurious velocities emerge at the contact-line region. FIG. 10(a) quantifies

556 the spurious velocity as ranging from 0.002-0.025 m/s. Furthermore, it is interesting that, compared with the hydrophilic contact angle of  $\theta = 45^{\circ}$ , the spurious velocity is mitigated with the 557 hydrophobic contact angle of  $\theta = 135^{\circ}$ . This is because, when the hydrophobic system reaches 558 559 equilibrium, the decreasing saturation in the first layer of the porous plate reduces the saturation 560 gradient and weakens the non-physical capillary force. The saturation extrapolation algorithm 561 enforces zero saturation gradients at the porous boundary based on Eqs. (18)–(19) so that the normal 562 to the gas-liquid interface  $n_{lg}$  is consistent with that of the conventional VOF approach. FIG. 8(b) 563 shows that the improved DBS model yields a contact angle that is almost identical to the prescribed 564 value, regardless of whether the configuration is hydrophobic or hydrophilic. Correspondingly, FIG. 565 9(b) shows that the spurious velocity of the improved DBS model is virtually zero if the contour 566 color bar is set with the same scale as the original DBS model. In quantitative comparison with the 567 original DBS model, FIG. 10(a) shows that the improved DBS model reduces the spurious velocity 568 by about one order of magnitude to less than  $10^{-3}$  m/s, which is close to the spurious velocity around 569 the gas-liquid interface far away from the contact line.



FIG. 9. Velocity fields of droplets on flat surfaces with different prescribed contact angles using: (a) original DBS and (b) improved DBS with saturation gradient correction. Solid white lines represent the gas–liquid interface ( $\alpha_1 = 0.5$  iso-surface).



FIG. 10. Spurious capillary number versus time: (a) droplets on flat surfaces simulated by the

original DBS and the improved DBS with saturation gradient correction, (b) droplets on curved surfaces simulated by the original DBS and the improved DBS with saturation gradient correction and smoothed norms.

570 Furthermore, a droplet on a curved surface is simulated to illustrate the influence of the 571 weighted smoothing scheme of the normal to the porous boundary on the contact-line dynamics 572 along a complex boundary. As discussed in Section III.C, the weighted smoothing scheme improves 573 the orthogonality of the normal to the porous boundary, which is approximated with a staircase mesh 574 in the micro-continuum model. Additionally, the weighted smoothing scheme constricts the nonzero 575 norm in the sharp vicinity of the porous boundary. By comparing the spurious velocity contours 576 obtained from the original and improved DBS models, FIG. 11 demonstrates that the spurious 577 velocity is significantly reduced by the weighted smoothing scheme, implying an improved force 578 balance at the curved contact line. Quantitatively, FIG. 10(b) shows that the spurious velocities are 579 reduced by one order of magnitude for contact angles of  $60^{\circ}$  and  $90^{\circ}$ , and by 70% for a contact 580 angle of 135°.



FIG. 11. Velocity fields of droplets on curved surfaces with different prescribed contact angles using: (a) original DBS and (b) improved DBS with the saturation gradient correction and the smoothed normal to the porous boundary. Solid white lines represent the gas–liquid interface ( $\alpha_l = 0.5$  iso-surface).

These results show that the improved DBS model achieves a more accurate contact angle than the original DBS model and reduces the spurious velocity by about one order of magnitude. These improvements are achieved by combining the correction scheme for the normal to the gas–liquid interface with the weighted smoothing scheme for the normal to the porous boundary.

585

## 586 C. Capillary rise

587 In terms of multiphase flow, this section simulates the capillary rise of a liquid through a narrow 588 tube using the original and improved micro-continuum DBS models, and compares the accuracy 589 against the conventional VOF model. The conventional VOF model is solved by the *interFoam* 590 solver. As shown in FIG. 12(a), the fluid domain extends over 1 mm × 20 mm and is discretized

with a uniform mesh of  $20 \times 400$ . On the left and right boundaries, the conventional VOF model

adopts the standard no-slip wall condition, while the micro-continuum model uses impermeable porous plates for approximations, as in Section IV.B. The fluid densities and viscosities are  $\rho_1 = 1000 \text{ kg/m}^3$  and  $\rho_g = 1 \text{ kg/m}^3$ ,  $v_1 = 10^{-6} \text{ m}^2/\text{s}$  and  $v_g = 1.48 \times 10^{-5} \text{ m}^2/\text{s}$ . The surface tension is  $\sigma = 0.07 \text{ kg/s}^2$ , and the contact angle on the wall or porous boundary is prescribed as 45°. The initial meniscus is set up about 2 mm lower than the analytical equilibrium height. The rising height reaches equilibrium when the vertical component of the surface tension force is balanced by the gravitational force of the risen liquid column, which can be analytically calculated as

591

$$h_{\rm eq} = \frac{2\sigma\cos\theta}{\Delta\rho|\mathbf{g}|d},\tag{32}$$

599 where *d* is the tube diameter and  $\Delta \rho = \rho_1 - \rho_g$  is the density difference between the gas and liquid 600 phases. The simulated equilibrium height is estimated as

$$\dot{h_{eq}} = \frac{\int_{S} \alpha_1 dS}{d} \,. \tag{33}$$

601 FIG. 12(a)-12(c) present the steady-state liquid saturation fields computed by the original DBS, 602 improved DBS, and conventional VOF models. FIG. 13(a) compares their equilibrium heights with 603 the analytical result. As can be observed, the equilibrium height predicted by the improved DBS 604 model shows the best agreement with the analytical result, with a relative error of -1.9%. The 605 original DBS and the conventional VOF models are comparable, both significantly underestimating 606 the equilibrium height with a relative error of -8.9%. Similar to the present results, some previous 607 studies have found that the conventional VOF model with the *interFoam* solver overpredicts the 608 contact angle and underestimates the equilibrium height.<sup>16</sup>

609 Furthermore, FIG. 12(d)-12(f) delineate the gas-liquid interfaces and highlight the spurious 610 velocities near the interface. The gas-liquid interface predicted by the original DBS model exhibits 611 noticeable deformation near the contact-line region. Even worse, considerable spurious velocities 612 appear near both the gas-liquid interface and contact-line region. However, the improved DBS 613 model largely eliminates the spurious currents, to even lower levels than the conventional VOF 614 model, due to the well-balanced surface tension force and the improved contact-line dynamics. For 615 a more intuitive analysis, FIG. 13(b) compares the spurious capillary numbers of the three 616 multiphase models. By comparison, the improved DBS model reduces the spurious velocity by at 617 least one order of magnitude compared with the conventional VOF model and by about two orders 618 of magnitude compared with the original DBS model. This benchmark demonstrates that the 619 improved DBS model can achieve minimal spurious capillary numbers of around 10<sup>-4</sup> when 620 multiphase flow dynamics are accounted for.



FIG. 12. Liquid saturation fields (*t*=2 s) for the capillary rise cases: (a) original DBS, (b) improved DBS, (c) conventional VOF; and velocity fields near the gas–liquid interface: (d) original DBS, (e) improved DBS, (f) conventional VOF. The gas–liquid interfaces are represented by white solid lines, and the analytical equilibrium height (9.91 mm) is represented by the yellow dotted lines.



FIG. 13. Comparison of different models over time: (a) simulated equilibrium height, (b) spurious capillary number.

621

## 622 **D.** Liquid drainage in a porous medium

In this section, pore-scale simulations of liquid drainage are performed to illustrate the applicability of the improved DBS model to capillary-dominated two-phase flow in complex porous media. This case is mainly concerned about pore-scale simulations of flow and transport in porous media, thus the effect of reservoir edge cannot directly affect the physics in such small-sized region. The computational domain is 960  $\mu$ m × 230  $\mu$ m in size and is meshed with a 960 × 230 Cartesian grid, and the pore size is about 50  $\mu$ m. For the micro-continuum model, the porosity is set to one in clean fluid regions and close to zero in the solid grains. This allows the solid grains to yield an

630 absolute permeability of  $10^{-16}$  m<sup>-2</sup> and reproduces the nonslip velocity condition on the surface by 631 penalization. To create the equivalent computational domain for the conventional VOF model, solid-632 grain-occupied cells are removed from the mesh and replaced by rectangular and triangular cells to 633 match the grain geometry via the OpenFOAM *snappyHexMesh* utility. The body-fitted grain surface 634 is then assigned as a nonslip boundary and shares the same wettability condition as the micro-635 continuum model. The computational domain is initially saturated with gas, denoted as "g," and 636 non-wetting liquid ( $\theta = 135^\circ$ ), denoted as "l," is injected from the left inlet at a velocity of

637  $v_0 = 0.005$  m/s. The fluid densities and viscosities are  $\rho_1 = 1000$  kg/m<sup>3</sup> and  $\rho_g = 20$  kg/m<sup>3</sup>,

638  $v_1 = 10^{-6} \text{ m}^2/\text{s}$  and  $v_g = 1.48 \times 10^{-5} \text{ m}^2/\text{s}$ . Surface tension values of  $\sigma = 0.005 \text{ kg/s}^2$ , 0.01 kg/s<sup>2</sup>, 639 and 0.05 kg/s<sup>2</sup> are used to produce inlet capillary numbers  $\text{Ca} = \mu_1 v_0 / \sigma$  ranging from  $10^{-3}$  to  $10^{-6}$ 640 <sup>4</sup>, allowing us to examine various spurious velocities and their impact on the multiphase flow 641 dynamics.

642 FIG. 14 presents the displacement pattern and saturation distribution at the end of the 643 simulation when the invading fluid reaches the other side of the computational domain, as solved 644 by the original DBS, improved DBS, and conventional VOF models. The gas-liquid displacement 645 produces a typical capillary fingering pattern. The injected liquid prefers to invade the larger pores 646 due to the lower entry capillary resistance. The fingering grows in both the longitudinal and lateral 647 directions, despite the longitudinal fingering proceeding slightly faster in this case. When Ca is 648 greater than  $10^{-4}$ , the three simulation results are similar, creating the same preferential pathways 649 and the same breakthrough at 50 ms. Some minor differences in the saturation distribution between 650 the micro-continuum and the conventional VOF models can be observed. This can be attributed to 651 the different mesh structures representing the solid grain geometry. Nevertheless, when Ca=10<sup>-4</sup>, the 652 leading fingering edge predicted by the original DBS model lags behind that simulated by the 653 improved DBS model and the conventional VOF model. The varying multiphase flow dynamics are 654 related to the presence of spurious currents, as shown in FIG. 15. The spurious currents can be 655 observed in the original DBS simulation result at  $Ca=5\times10^{-4}$ , and become significantly intensified 656 at Ca=10<sup>-4</sup>. From the magnified views of the local saturation and velocity fields for Ca=10<sup>-4</sup> in FIG. 657 16, the spurious velocities presented in the original DBS results are much more remarkable than the 658 physical velocity, particularly at the corner-line regions. Quantitative comparisons in FIG. 17 659 indicate that the improved DBS model substantially reduces the spurious velocity by one order of 660 magnitude to a level comparable to the conventional VOF model. These observations suggest that 661 the improved DBS model can accurately simulate the multiphase flow dynamics in the capillary-662 dominated regime at  $Ca \sim 10^{-4}$  due to the limited spurious velocity, even in complicated porous 663 media. Regarding the comparable simulations to the conventional VOF model, the improved

664 contact-line dynamics given by the correction scheme of the normal to the gas-liquid interface and
665 the weighted smoothing scheme of the normal to the porous boundary play an essential role in
666 limiting the spurious velocities.



FIG. 14. Displacement patterns at breakthrough (t=50 ms) for different capillary numbers using: (a) original DBS model, (b) improved DBS model, and (c) conventional VOF model.



FIG. 15. Velocity fields (*t*=50 ms) for different capillary numbers using: (a) original DBS model,(b) improved DBS model, and (c) conventional VOF model.



FIG. 16. Magnified views of local saturation and velocity fields (t=50 ms) for an inlet capillary number of Ca=10<sup>-4</sup> using: (a) original DBS model, (b) improved DBS model, and (c) conventional VOF model. White lines represent the gas–liquid interface and black arrows quantify the magnitude and direction of velocity vectors.



FIG. 17. Time-dependent spurious capillary number based on the maximum velocity calculated by the original DBS model, improved DBS model, and conventional VOF model: (a)  $Ca=10^{-3}$ , (b)  $Ca=5\times10^{-4}$ , (c)  $Ca=10^{-4}$ .

667 These four illustrative cases show the ability of the improved DBS model to simulate capillary-668 dominated multiphase flows at the pore scale. During verification, some benchmark results were 669 provided by the conventional VOF model, implying that the micro-continuum model can 670 successfully recover known multiphase Navier-Stokes solutions when used as a pore-scale model. Not limited to the pore scale, previous studies<sup>14, 16</sup> have clearly demonstrated that the micro-671 672 continuum model has the ability to simulate multiphase Darcy flows when used as a continuum-673 scale model and multiscale multiphase dynamics when used as a hybrid-scale model. The 674 contribution of the present study is the development of an improved DBS model in mitigating 675 spurious velocities, leading to an enhanced capacity in the capillary-dominated regime. In further 676 work, multiphase reactive transport flows with heterogeneous reactions in porous media, such as 677 hydrate dissociation, will be investigated to demonstrate that the improved DBS model has the 678 capacity to solve complex multiscale problems, typically with capillary numbers of around  $10^{-4}$ .

679

## 680 V. CONCLUSIONS

681 The present study has improved the multiphase micro-continuum DBS model to enable 682 accurate simulations of two-phase flows at capillary numbers as low as 10<sup>4</sup>. A hybrid interpolation 683 scheme was proposed to improve the accuracy of the normal to the gas-liquid interface and the 684 interface curvature. At the porous boundary, the normal to the gas-liquid interface was revised by a 685 saturation extrapolation scheme to exclude the impact of saturation in the unresolved porous regions 686 on the contact angle correction. To further guarantee the accurate contact angle correction at the 687 curved surface, a weighted smoothing scheme was constructed to enhance the orthogonal property 688 of the normal to the porous boundary and constrain the nonzero norm at the porous boundary. 689 Compared with the original DBS model,<sup>16</sup> the combination of these three schemes theoretically 690 improves the force balance and mitigates the spurious velocities at the gas-liquid interface and 691 contact lines.

692 Four benchmark cases were investigated to verify the numerical performance of the improved 693 DBS model. First, the impact of different interpolation schemes for the normal to the gas-liquid 694 interface on the interfacial dynamics was investigated by simulating a static gas bubble in liquid. The IG interpolation scheme used in the interFoam<sup>51</sup> and hybridPorousInterFoam<sup>16</sup> solvers was 695 696 found to underestimate the interface curvature and surface tension force, leading to a convex gasliquid interface. Conversely, the IN interpolation scheme used in the poreFoam9, 44 and 697 698 interGCFoam<sup>52</sup> solvers overpredicted the interface curvature and surface tension force, resulting in 699 a sunken gas-liquid interface. The hybrid interpolation scheme eliminated the interface deformation 700 and robustly reduced the spurious velocity at the gas-liquid interface by one or two orders of 701 magnitude compared with the IG or IN scheme. Second, stationary droplets on flat and curved 702 surfaces were simulated. The results prove that the improved DBS model has the ability to target 703 the prescribed contact angle and decrease the spurious velocity at the contact-line region by about 704 one order of magnitude compared with the original DBS model. In the third and fourth examples, 705 capillary rise and liquid drainage in a porous medium were simulated to demonstrate that the 706 improved DBS model can simulate capillary-dominated multiphase flows with negligible spurious 707 velocities at Ca=10<sup>-4</sup> in simple and complex geometries, respectively.

The improved model effectively reduces the spurious velocity for capillary-dominated multiphase flow to the order of the traditional VOF method using the body-fitted meshes. However, the computational efficiency of the DBS model is still not good enough. For example, the fourth test case, which involves multiphase flow in a porous medium meshing 69600 grid blocks, requires 64 CPU cores to complete the computation in about 20 minutes for a physical time of 0.05 seconds.

In future work, the improved DBS model needs more physics incorporations to simulate the multiphase reactive flows within multiscale structures. And the computational efficiency will be improved by removing unused solid phases from the computational domain and optimizing the solver algorithms. After verifying the improved DBS method with other multiscale solvers and experimental results, hybrid-scale simulations will be performed on specific scenarios including carbonate dissolution and methane hydrate dissociation, to understand the effect of sub-resolution porosity on multiphase reactive flow in the natural multiscale rock.

720

# 721 SUPPLEMENTARY MATERIAL

The boundary conditions and simulation parameters of the validation cases can befound in the Supplementary Material.

724

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729	
730	DECLARATION OF INTERESTS
731	The authors declare that they have no known competing financial interests or personal
732	relationships that could have appeared to influence the work reported in this paper.
733	
734	DATA AVAILABILITY STATEMENT
735	The data that support the findings of this study are available from the corresponding author
736	upon reasonable request.
737	
738	AUTHOR CONTRIBUTIONS
739	Zhiying Liu: Conceptualization (lead); Methodology (lead); Validation (equal); Writing - original
740	draft (lead).
741	Junyu Yang: Conceptualization (supporting); Methodology (supporting); Validation (equal).
742	Qianghui Xu: Writing - original draft (supporting); Writing - review and editing (equal);
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745	
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(a)	(b)					(c)						
1 1 1 1 -0 0	1	1	1	1	-0	o	1	1	1	1	-0	0
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