## Effect of hydraulic fracture deformation hysteresis on CO<sub>2</sub> huff-n-puff performance in shale gas reservoirs

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## S1 Multi-component flow model and geomechanics equations discretization

## S1.1 Multi-component flow model

 $K_n$  is the Knudsen number, and  $\alpha_K$  is the rarefaction coefficient, they are defined as (Song et al., 2016; Fan et al., 2019; Lijun et al., 2019):

$$K_{\rm n} = \frac{\lambda}{r_{\rm h}}, \quad \alpha_{\rm K} = \frac{1.358}{1 + 0.170 K_{\rm n}^{-0.4348}}$$
 (S1)

where  $\lambda$  is the mean free paths of gas molecules, and  $r_h$  is the pore radius (Song et al., 2016).

$$\lambda = \frac{\mu}{p} \sqrt{\frac{\pi z R T}{2M_g}}, \quad r_h = 2\sqrt{2\tau_0} \sqrt{\frac{k_\infty}{\phi_0}}$$
(S2)

where z is the gas compressibility factor; T is the reservoir temperature; R is the universal gas constant;  $M_g$  is the gas molar weight;  $\tau_0$  is the initial tortuosity, and  $\phi_0$  is the initial porosity.

## S1.2 Geomechanics equations discretization

In this study, we added the Heaviside fracture tip asymptotic and junction enrichment functions to the standard finite element space for simulating the displacement discontinuity at hydraulic fractures. Then, the expression of the enriched displacement field is given as

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{i \in I} N_i(\boldsymbol{x}) \boldsymbol{u}_i + \sum_{j=1}^{N_{\text{dis}}} \sum_{i \in I^{\text{dis}}} N_i(\boldsymbol{x}) (H(\boldsymbol{x}) - H(\boldsymbol{x}_i)) \boldsymbol{a}_i + \sum_{k=1}^{N_{\text{tip}}} \sum_{i \in I^{\text{tip}}} N_i(\boldsymbol{x}) \sum_{\alpha=1}^{4} (F_{\text{tip}}^{\alpha}(\boldsymbol{x}) - F_{\text{tip}}^{\alpha}(\boldsymbol{x}_i)) \boldsymbol{b}_i^{\alpha} + \sum_{l=1}^{N_{\text{jun}}} \sum_{i \in I^{\text{jun}}} N_i(\boldsymbol{x}) (J(\boldsymbol{x}) - J(\boldsymbol{x}_i)) \boldsymbol{c}_i$$
(S3)

where *I* denotes the node set of a grid; subscript *i* denotes the *i*-node; *N* is the standard shape function;  $I^{\text{dis}}$ ,  $I^{\text{tip}}$ , and  $I^{\text{jun}}$  are the node subsets to enrich for the fracture discontinuity, tip and junction, respectively;  $N_{\text{dis}}$ ,  $N_{\text{tip}}$ , and  $N_{\text{jun}}$  are the numbers of fractures, fracture tips and fracture junctions, respectively; *u*, *a*, *b*, and *c* are the standard and additional degrees of freedom (DOFs), respectively; *H*, *F*, and *J* represent the Heaviside function, fracture tip asymptotic function and junction function, respectively (Khoei, 2014). For convenience, Eq. S3 can be written as

$$\boldsymbol{u}(\boldsymbol{x}) = N_{u}^{u}(\boldsymbol{x})\boldsymbol{u} + N_{u}^{a}(\boldsymbol{x})\boldsymbol{a} + N_{u}^{b}(\boldsymbol{x})\boldsymbol{b} + N_{u}^{c}(\boldsymbol{x})\boldsymbol{c}$$
(S4)

where,  $N_u^u(x)$ ,  $N_u^a$ ,  $N_u^b$ , and  $N_u^c$  are the matrix of the standard and enriched shape functions, respectively. Therefore, the corresponding strain vector is given by

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{B}_{u}^{u}(\boldsymbol{x})\boldsymbol{u} + \boldsymbol{B}_{u}^{a}(\boldsymbol{x})\boldsymbol{a} + \boldsymbol{B}_{u}^{b}(\boldsymbol{x})\boldsymbol{b} + \boldsymbol{B}_{u}^{c}(\boldsymbol{x})\boldsymbol{c}$$
(S5)

where  $B_u^u(x) = LN_u^u(x)$ ,  $B_u^a(x) = LN_u^a(x)$ ,  $B_u^b(x) = LN_u^b(x)$ ,  $B_u^c(x) = LN_u^c(x)$ , and L indicates the matrix differential operator

$$\boldsymbol{L} = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial z \\ \partial/\partial y & \partial/\partial x & 0 \\ 0 & \partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & \partial/\partial x \end{bmatrix}$$
(S6)

Now, we substitute Eqs. S4 and S5 into Eq. 15, and consider that Eq. 15 must apply for any kinematically admissible test function, then Eq. 15 is written as

$$f_{\alpha}^{\text{int}} = f_{\alpha}^{\text{ext}}, \quad \alpha = u, a, b, c$$
 (S7)

with

$$\boldsymbol{f}_{\alpha}^{\text{int}} = \int_{\Omega} \left( \boldsymbol{B}_{u}^{\alpha} \right)^{\mathrm{T}} \boldsymbol{C}_{a} \boldsymbol{\varepsilon} \mathrm{d}\boldsymbol{\Omega}$$
(S8)

$$f_{\alpha}^{\text{ext}} = \int_{\Omega} \left( \boldsymbol{B}_{u}^{\alpha} \right)^{\mathrm{T}} \boldsymbol{m} p_{a} \, \mathrm{d}\Omega + \int_{\Gamma_{\text{HF}}} \left[ \left[ \boldsymbol{N}_{u}^{\alpha} \right] \right]^{\mathrm{T}} \left( p_{\text{HF}} + \sigma_{n} \right) \cdot \boldsymbol{n}_{\text{HF}} \, \mathrm{d}\Gamma + \int_{\Omega} \left( \boldsymbol{N}_{u}^{\alpha} \right)^{\mathrm{T}} \boldsymbol{f} \, \mathrm{d}\Omega + \int_{\Gamma_{\text{t}}} \left( \boldsymbol{N}_{u}^{\alpha} \right)^{\mathrm{T}} \boldsymbol{\bar{t}} \, \mathrm{d}\Gamma \\ \underbrace{- \int_{\Gamma_{\text{HF}}} \frac{\tau}{2M} \left( -\frac{\partial \sigma_{n}}{\partial \varepsilon_{n}} \frac{\boldsymbol{n}_{\text{HF}}}{\boldsymbol{d}_{\text{HF0}}} \right) \cdot \left( \left[ \left[ \boldsymbol{N}_{u}^{\alpha} \right] \right] - \Pi \left[ \left[ \boldsymbol{N}_{u}^{\alpha} \right] \right] \right)^{\mathrm{T}} \left( \sigma_{n} - \Pi \sigma_{n} \right) \mathrm{d}\Gamma} \underbrace{\text{Stabilizing term}}$$
(S9)

where  $\mathbf{f}^{int}$  and  $\mathbf{f}^{ext}$  represent the internal and external force vectors;  $\mathbf{m} = [1, 1, 1, 0, 0, 0]^{T}$ .