

1 **MRST-Shale: an open-source framework for generic numerical modeling of**  
2 **unconventional shale and tight gas reservoirs**

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5 **Highlights**

- 6
- 7 • A generic numerical model for shale gas flow in tight reservoir is proposed
  - 8 • A flexible open-source framework OpenShale is developed with EDFM
  - 9 • EDFM can lead to large error for shale gas flow without help of grid refinement
  - 10 • A new geomechanics model for hydraulic and natural fractures is proposed and evaluated
  - 11 • OpenShale successfully applied in field history matching and new model evaluation

12 **Abstract**

13 We present a generic and open-source framework for the numerical modeling of the expected  
14 transport and storage mechanisms in unconventional gas reservoirs. These unconventional reservoirs  
15 typically contain natural fractures at multiple scales. Considering the importance of these fractures in  
16 shale gas production, we perform a rigorous study on the accuracy of different fracture models. The  
17 framework is validated against an industrial simulator and is used to perform a history-matching  
18 study on the Barnett shale.

19 This work presents an open-source code that leverages cutting-edge numerical modeling capabilities  
20 like automatic differentiation, stochastic fracture modeling, multi-continuum modeling and other  
21 explicit and discrete fracture models. We modified the conventional mass balance equation to  
22 account for the physical mechanisms that are unique to organic-rich source rocks. Some of these  
23 include the use of an adsorption isotherm, a dynamic permeability-correction function, and an  
24 embedded discrete fracture model (EDFM) with fracture-well connectivity. We explore the accuracy  
25 of the EDFM for modeling hydraulically-fractured shale-gas wells, which could be connected to  
26 natural fractures of finite or infinite conductivity, and could deform during production.

27 Simulation results indicates that although the EDFM provides a computationally efficient model for  
28 describing flow in natural and hydraulic fractures, it could be inaccurate under these three  
29 conditions:

- 30
- 31 1. when the fracture conductivity is very low
  - 32 2. when the fractures are not orthogonal to the underlying Cartesian grid blocks, and
  - 33 3. when sharp pressure drops occur in large grid blocks with insufficient mesh refinement.

34 Each of these results are very significant considering that most of the fluids in these ultra-low matrix  
35 permeability reservoirs get produced through the interconnected natural fractures, which are  
36 expected to have very low fracture conductivities. We also expect sharp pressure drops near the

1 fractures in these shale gas reservoirs, and it is very unrealistic to expect the hydraulic fractures or  
2 complex fracture networks to be orthogonal to any structured grid. In conclusion, this paper presents  
3 an open-source numerical framework to facilitate the modeling of the expected physical mechanisms  
4 in shale-gas reservoirs. The code was validated against published results and a commercial simulator.  
5 We also performed a history-matching study on a naturally-fractured Barnett shale-gas well  
6 considering adsorption, gas slippage & diffusion and fracture closure as well as proppant embedment,  
7 using the framework presented.

8 This work provides the first open-source code that can be used to facilitate the modeling and  
9 optimization of fractured shale-gas reservoirs. To provide the numerical flexibility to accurately  
10 model stochastic natural fractures that are connected to hydraulically-fractured wells, it is built atop  
11 other related open-source codes. We also present the first rigorous study on the accuracy of using  
12 EDFM to model both hydraulic fractures and natural fractures that may or may not be  
13 interconnected.

14 Source code is available at [https://github.com/BinWang0213/MRST\\_Shale](https://github.com/BinWang0213/MRST_Shale)

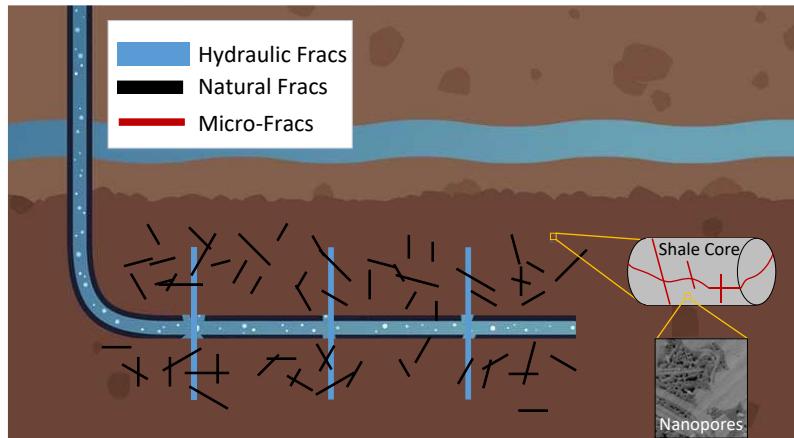
15 **Key words:** Shale gas; MRST; embedded discrete fracture model; Open-source implementation

## 16 1 Introduction

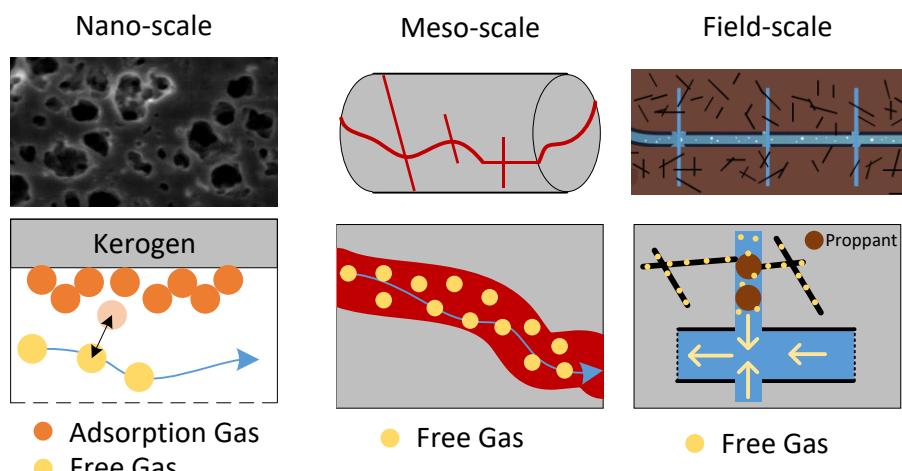
17 Unconventional gas resources gain great interest recently due to successful economic development  
18 and strong energy supply around the world. Advancement of horizontal well drilling and hydraulic  
19 fracturing technology as well as better understanding unconventional reservoirs drives substantial  
20 growth of shale gas production (Bowker, 2007). Unlike conventional reservoirs, unconventional  
21 shale gas reservoirs can be characterized by ultra-low permeability, low porosity, complex transport  
22 mechanism and multi-scale fractures (Akkutlu et al, 2018). Development of unconventional  
23 resources is more technology-demanding and expensive. Thus, accurate modeling and numerical  
24 simulation of shale gas flow is critical for evaluating, designing and managing stimulation and  
25 production processes.

26 Well-established flow and transport theory for conventional reservoir rocks are not directly  
27 applicable to unconventional porous media (Gensterblum et al, 2015). For decades, researchers have  
28 been investigating the storage and transport mechanisms for unconventional reservoirs, which  
29 includes gas desorption, adsorbed gas porosity, gas slippage, and Knudsen diffusion, etc (Javadpour  
30 et al, 2007; Wang and Reed, 2009; Civan et al, 2010,2011; Sakhaei and Bryant, 2012; Akkutlu and  
31 Fathi, 2012, Yu et al, 2016 and Tan et al, 2018). In addition, the fractured shale matrix is comprised  
32 of a hierarchical network of pores down to a few nanometers, cracks and micro-fractures, which

1 makes the formation a multi-scale porous medium with large heterogeneity and anisotropy (Akkutlu  
 2 et al, 2018). Hence, the complex gas transport mechanisms and multiscale fracture system (**Figs. 1-2**)  
 3 pose a great challenge to accurately and efficiently evaluate and simulate well performance in shale  
 4 gas reservoirs.



5 **Fig 1 – Multi-scale nature of shale gas production**



6 **Fig 2 – Multi-scale shale gas storage and transport**

7  
 8 In recent years, significant efforts have been made to model gas flow in unconventional  
 9 reservoirs. These methods can be categorized into analytical model, semi-analytical model and  
 10 numerical simulations. The analytical method dates back to 1970s, where the line-source  
 11 fundamental solution is derived for simple fracture geometry such as single bi-wing hydraulic  
 12 fractures and pseudo-pressure is applied to linearized the non-linear real gas equation (Gringarten et  
 13 al, 1974, Cinco et al, 1978 and Agarwal 1979). Recently, the analytical method is extended into  
 14 semi-analytical method to consider complex fracture networks and shale gas storage mechanism  
 15 based on the boundary element method (Zuo et al, 2016, Chen et al, 2015, 2016, 2017, 2018; Yang et  
 16 al, 2018).

1 al, 2016a, 2016b, 2017, Yu et al, 2016b, 2017 and Li et al, 2018). Although analytical-based method  
 2 is fast and accurate, it is difficult to handle rock heterogeneity, multi-phase, multi-compositional and  
 3 strong non-linear transport mechanisms in shale gas flow problems (Houze et al, 2010 and Olorode  
 4 et al, 2013). On the other hand, numerical simulation has been proven to be is the most general and  
 5 rigorous method to account for arbitrary non-linear physics and fracture geometry for unconventional  
 6 reservoirs (Olorode et al, 2013,2017 and Cipolla et al, 2012). Highly coupled non-linear physics and  
 7 treatment of multi-scale fractured system are two key issues in shale gas flow simulation. Fully  
 8 implicit scheme with Automatic Differentiation (AD) is a robust and generic method to solve the  
 9 highly coupled non-linear problem accurately and efficiently (Zhou et al, 2011 and Krogstad et al,  
 10 2015). In terms of multi-scale fractured system, dual continuum method (Warren and Root, 1963)  
 11 and discrete fracture method (Karimi-fard et al, 2004, Hoteit and Firoozabadi, 2005, Hajibeygi et al,  
 12 2011 and Moinfar et al, 2014) are generally used to model highly connected fractures and long,  
 13 disconnected hydraulic/natural fractures (Fig. 1), respectively. A hierarchical method is also proposed  
 14 by integrating continuum method and discrete fracture method for multi-scale fractured system  
 15 where the micro-fractures are upscaled into matrix permeability tensor and hydraulic/natural  
 16 fractures are modeled explicitly (Lee et al, 2001 and Karimi-Fard et al, 2006). Unstructured gridding  
 17 with local grid refinement (LGR) is generally used to capture the irregular fracture geometry and  
 18 sharp pressure gradient near the fractures. However, it is are still challenging to generate conforming  
 19 mesh efficiently for complex fracture networks (Karimi-Fard, Durlofsky, 2016). Recently, an  
 20 embedded discrete fracture model is developed to resolve the complex gridding issue. Using EDFM,  
 21 the complex fractures are embedded in conventional matrix grids without conforming the matrix  
 22 grids with fracture plane, thus it is more efficient for complex fracture networks. In addition, it can  
 23 be easily integrated into well-established reservoir simulator without accessing the code (Xu, 2015  
 24 and Olorode et al, 2017). **Table 1** shows the advantages and disadvantages of these method where  
 25 unstructured grid and EDFM are the two most promising methods for generic shale gas simulation  
 26 with multi-scale fractures.

27 **Table 1. Comparison of shale gas flow simulation methods**

	Analytical	Semi-analytical	Structured grid	Unstructured grid	EDFM
Accuracy	++	++	+++	+++	++
Nonlinear mechanisms*	+	+	+++	+++	+++
Rock heterogeneity	+	+	+++	+++	+++

Fracture gridding	+++	+++	+	+	+++
Preprocessing <sup>**</sup> efficiency	+++	+++	+++	+++	++
Computational <sup>***</sup> efficiency	+++	+++	+	++	++

\* Nonlinear gas transport & storage model , multi-phase flow, compositional flow

\*\* 2D/3D geometry calculations, such plane-plane intersection, point-plane distance

\*\*\* linear algebra and Newton's calculations

1 Flow and transport theory and models for unconventional reservoir is a rapid evolving area of  
2 research, many of the existing and newly discovered phenomenon have not been completely  
3 understood. Also, the effect of these mechanism on practical well performance is not clear. To the  
4 best of our knowledge, almost all existing numerical models for shale gas reservoir are implemented  
5 in in-house simulators or commercial simulators (Jiang and Younis, 2015, Cao et al, 2016, Xu et al,  
6 2017, Wang et al, 2017 and Akkutlu et al, 2018). Hence, it is necessary to develop a flexible and  
7 generic open-source framework to fill this gap.

8 In this paper, a generic numerical model is developed to simulate shale gas flow in  
9 unconventional reservoirs with multi-scaled fractures, which can be used to integrate any shale gas  
10 transport and storage mechanism for unconventional reservoirs as well as the geomechanics effect  
11 for fracture system. An efficient and flexible framework (OpenShale) is also developed using an  
12 open-source reservoir simulation toolkit (MRST) and EDFM. OpenShale can handle **deterministic**  
13 hydraulic fractures and stochastic natural fractures with arbitrary geometry and distribution. The  
14 framework is firstly verified against **a** commercial simulator and **an** in-house reservoir simulator that  
15 **employs** unstructured grid **to simulate** shale gas transport with non-planar hydraulic fracture, gas  
16 desorption, gas slippage & diffusion. The advantages and limitation of EDFM for shale gas flow  
17 problem is also discussed. Finally, field application of history matching and new geomechanics  
18 model evaluation are **studied**.

## 19 2 Mathematical equations

20 Considering the isothermal single-component single-phase gas flow in 2D fractured porous  
21 media with 1D fracture line without gravity effect. The general governing equation for shale gas flow  
22 in matrix ( $\Omega_m$ ), considering storage ( $m_{ad}$ ) and transport mechanisms ( $F_{app}$ ), can be expressed as  
23 follows:

$$24 \quad \frac{\partial}{\partial t} (\rho_g \phi + (1-\phi)m_{ad}) + \nabla \cdot (-\rho_g \frac{\prod_i F_{app,i} k_0}{\mu_g} \nabla p) = \rho_g q_w \quad \text{in } \Omega_m \quad (1)$$

1      Similarly, the governing equation for fracture ( $\Omega_f$ ), only considering transport mechanisms,

2      can be expressed as follows:

$$3 \quad \frac{\partial}{\partial t} (\rho_g \phi) + \nabla \cdot (-\rho_g \frac{\prod_i F_{app,i} k_0}{\mu_g} \nabla p) = \rho_g q_w \quad \text{in } \Omega_f \quad (2)$$

4      Introducing inverse formation volume factor  $b_g = \rho_g / \rho_{gsc}$  ( $\rho_g = b_g \rho_{gsc}$ ), the above equation

5      can be rewritten as follows:

$$6 \quad \begin{aligned} & \frac{\partial}{\partial t} \left( b_g \phi + \frac{(1-\phi)}{\rho_{gsc}} m_{ad} \right) + \nabla \cdot \left( -b_g \frac{\prod_i F_{app,i} k_0}{\mu_g} \nabla p \right) = b_g q_w \quad \text{in } \Omega_m \\ & \frac{\partial}{\partial t} (b_g \phi) + \nabla \cdot \left( -b_g \frac{\prod_i F_{app,i} k_0}{\mu_g} \nabla p \right) = b_g q_w \quad \text{in } \Omega_f \end{aligned} \quad (3)$$

7      where  $\rho_g$  is the mass density of gas, M/L<sup>3</sup>;  $\mu_g$  is the dynamic viscosity of natural gas, N.T/L<sup>2</sup>;  $m_{ad}$   
8      is the accumulation term due to adsorption, M/L<sup>3</sup>;  $\phi$  is the matrix porosity, dimensionless;  $k_0$  is the  
9      absolute Darcy permeability of the reservoir rock, L<sup>2</sup>.  $F_{app,i}$  is the  $i$ -th permeability correction factor  
10     for a specific shale gas transport mechanism;  $q_w$  is the volumetric sink/source term, M/L<sup>3</sup>/T.  $k_0$  is the  
11     absolute Darcy permeability of the reservoir rock, L<sup>2</sup>.

## 12     2.1 Gas properties

13     *Density*: The pressure-dependent density of natural gas can be calculated by the real gas law:

$$14 \quad \rho_g = \frac{pM}{Z(p,T)RT} \quad (4)$$

15     where  $M$  is the molecule weight of the natural gas, M/Mol;  $R$  is the Boltzmann constant, 8.314

16     ML<sup>2</sup>T<sup>-2</sup>/T/mole);  $T$  is the reservoir temperature, T;

17     The compressibility factor  $Z$  can be calculated using either implicit Peng-Robinson  
18     equation-of-state (PR-EOS) equation or empirical explicit equation. Using the empirical equation,  
19     the complex natural gas mixture can be considered as a single component with pseudo-temperature  
20     and pseudo-pressure. Mahmoud (2014) developed an explicit empirical equation for natural gas  
21     mixture as follows:

$$22 \quad Z(p,T) = 0.702e^{-2.5T_{pr}} \cdot p_{pr}^2 - 5.524e^{-2.5T_{pr}} \cdot p_{pr} + (0.044T_{pr}^2 - 0.164T_{pr} + 1.15) \quad (5)$$

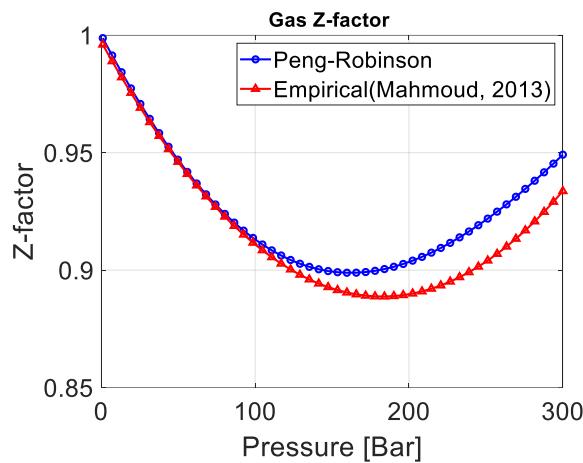
23     where the reduced-temperature and reduced-pressure can be expressed as  $T_{pr} = T / T_c$  and

$p_{pr} = p / p_c$ , respectively.  $T_{pc}$  and  $P_{pc}$  are the pseudo-critical pressure and pseudo-critical temperature for the shale gas mixture, respectively.

Also, for single component gas simulation, such as methane, the Z factor can be accurately estimated by solving a cubic function of PR-EOS as follows (Lira and Elliott, 2012):

$$\begin{aligned} Z^3 + a_2 Z^2 + a_1 Z + a_0 &= 0 \\ a_0(p, T) &= (AB - B^2 - B^3), \quad a_1(p, T) = A - 3B^2 - 2B, \quad a_2(p, T) = B - 1 \\ A &= ap / (RT)^2, \quad B = bp / (RT) \\ a &= \frac{0.457235R^2T_c^2}{p_c}, \quad b = \frac{0.0777961RT_c}{p_c} \end{aligned} \quad (6)$$

In this paper, an analytical solution (see details in appendix B of Lira and Elliott, 2012) is used for solving the cubic equation. For more complex natural gas mixture, it requires complex flash calculation and belongs multi-component compositional simulation which will be investigated in our future work. **Fig. 3** shows an estimation of Z-factor for methane using Eq.5 and Eq. 6, respectively.



**Fig. 3 Evaluated natural gas Z-factor for empirical and PR-EOS models with  $T=352$  K,  $T_c=191$  K,  $p_c=4.64$  MPa,  $R=8.314$  J/(K.mol)**

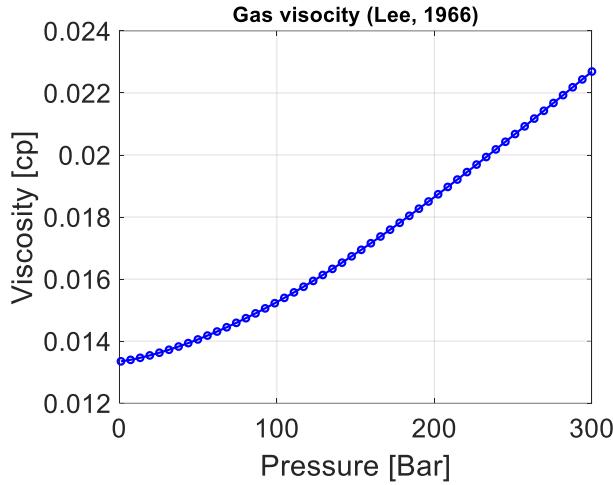


Fig. 4 Evaluated natural gas viscosity using Lee Lee-Gonzalez-Eakin empirical correlation with  $M=16.04$  g/mol and  $T=633.6$  Rankine

Viscosity: The density-dependent viscosity of natural gas can be estimated by Lee-Gonzalez-Eakin empirical correlation (Lee et al, 1966) as follows:

$$\mu_g = 10^{-7} K \exp(X \rho_g^Y)$$

$$K = \frac{(9.379 + 0.01607M)T^{1.5}}{209.2 + 19.26M + T}, \quad X = 3.448 + \frac{986.4}{T} + 0.01009M, \quad Y = 2.447 - 0.2224X \quad (7)$$

where the unit of  $M$ ,  $T$  are g/mol and Rankine, respectively. Fig. 4 shows an estimation of viscosity for methane using Eq.7.

Noted that although the usage of pseudo-pressure equation can eliminate the nonlinearity issue introduced by pressure-dependent gas viscosity and compressibility (Eqs. 5-6), it leads lead to even larger errors especially for tight shale reservoirs (Houze et al, 2010). Thus, in this paper, the real-gas equation is used.

## 2.2 Transport and storage mechanism

Since rapid commercial development of unconventional tight reservoirs in recent years, many researchers spend enormous effort to understand the transport and storage mechanism of shale gas in such complex multi-scale systems (Figs. 1-2). Several key physical mechanisms (Yu et al, 2016; Klinkenberg, 1941; Florence et al, 2007; Javadpour, 2007; Civan, 2010) can be summarized as in Table 2.

In the presented open-source code, *OpenShale*, any storage and transport mechanisms models can be easily implemented via defining nonlinear gas storage function ( $m_{ad}$ ) and permeability correction function ( $F_{app}$ ). Demonstrative storage and transport models implemented in OpenShale

1 this study are shown as follows:

2 **Table 2. Key transport and storage mechanism for shale gas flow**

Mechanism	Models	Type	Continuum
Adsorption	Langmuir, BET	S*	Matrix
Slip flow & Diffusion	Klinkenberg, Florence, Javadpour, Civan	T*	Matrix
Non-Darcy flow	Darcy-Forchheimer	T	Fracture

\*S-Storage mechanism, T-Transport mechanism

3 *Adsorption*: The gas molecules adsorbed in the pore wall of Kerogen in shale reservoir can be  
 4 modeled using monolayer Langmuir isotherm and multiple layer BET isotherm as follows (Yu et al,  
 5 2016a):

6

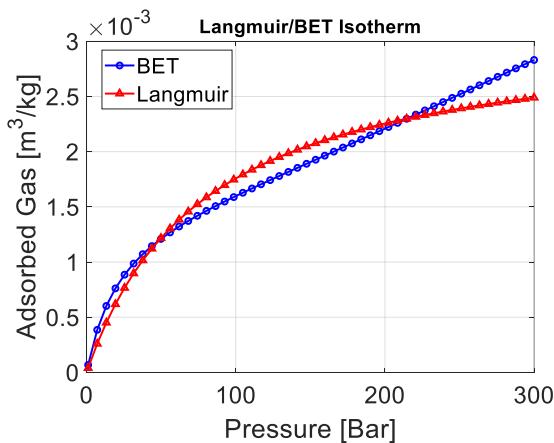
$$\text{Langmuir: } m_{ad} = \rho_s \rho_{gsc} \frac{pV_L}{p + P_L} \quad (8)$$

7

$$\text{BET: } m_{ad} = \rho_s \rho_{gsc} \frac{V_m C p_r}{1 - p_r} \left[ \frac{1 - (n+1)p_r^n + np_r^{n+1}}{1 + (C-1)p_r - Cp_r^{n+1}} \right] \quad (9)$$

$$p_r = \frac{p}{P_s}, \quad P_s = \exp(7.7437 - \frac{1306.5485}{19.4362 + T})$$

8 where  $V_L$  is the Langmuir volume,  $\text{L}^3/\text{M}$ .  $P_L$  is the Langmuir pressure,  $\text{M/L/T}^2$ .  $\rho_s$  is the density  
 9 of rock bulk matrix  $\text{M/L}^3$ ,  $V_L$  is the Langmuir volume (the maximum adsorption capacity at a given  
 10 temperature),  $\text{L}^3/\text{M}$ .  $P_L$  is the Langmuir pressure (the pressure at which the adsorbed gas volume is  
 11 equal to  $V_L/2$ ),  $\text{M/L/T}^2$ .  $V_m$  is the BET adsorption volume,  $\text{L}^3/\text{M}$ .  $C$  is the BET adsorption constant,  
 12 dimensionless.  $n$  is the BET adsorption molecular layers, dimensionless.  $p_s$  is the pseudo-saturation  
 13 pressure,  $\text{M/L/T}^2$ . Noted that, the unit of  $P_s$  is MPa. **Fig. 5** shows an estimation of adsorption  
 14 isotherm using Eq.8 and Eq. 9, respectively.



1      **Fig. 5 Langmuir and BET isotherms curve with  $V_L=0.0031 \text{ m}^3/\text{kg}$  and  $P_L=7.89 \text{ MPa}$ ,**  
 2       **$T=327.59 \text{ K}$ ,  $P_s=53.45 \text{ MPa}$ ,  $V_m=0.0015 \text{ m}^3/\text{kg}$ ,  $C=24.56$  and  $n=4.46$**

3      *Slippage flow & Diffusion:* Considering slippage and diffusion effect of shale gas flow in the  
 4      matrix, the apparent permeability in the low-pressure region around the fracture will be increased. In  
 5      the OpenShale, the Florence's (2007) permeability correction factor (**Fig. 4**) is implemented as  
 6      follows:

7                          
$$F_{app} = (1 + \alpha K_n)(1 + \frac{4K_n}{1 + K_n}) \quad (10)$$

8                          
$$K_n = \frac{\mu_g}{2.8284 p_g} \sqrt{\frac{\pi R T}{2M} \frac{\phi}{k_0}} \quad (11)$$
  

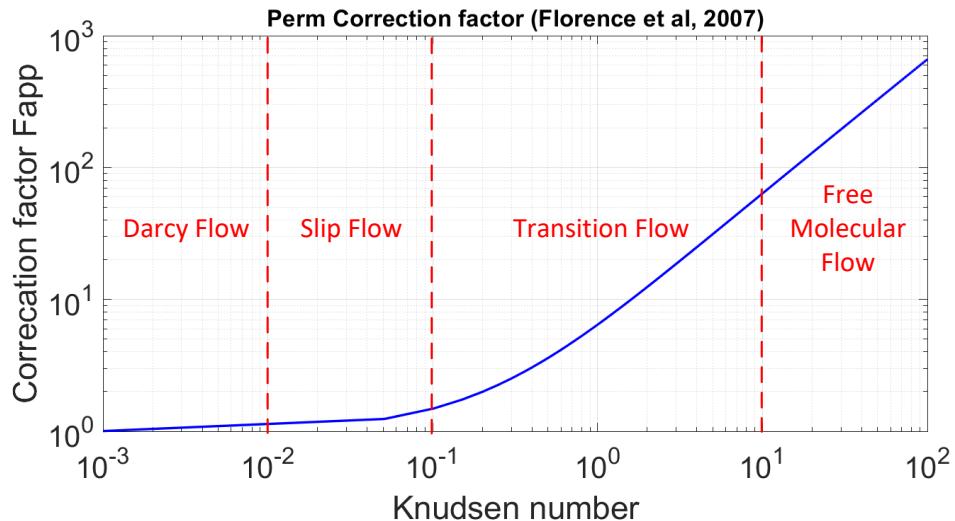
$$\alpha = \frac{128}{15\pi^2} \tan^{-1}(4K_n^{0.4})$$

9      where  $Kn$  is the Knudsen number, dimensionless.  $\alpha$  is the rarefaction parameter, dimensionless.

10     **Fig. 6** shows an estimation of gas slippage and diffusion permeability correction factor for methane  
 11    using Eqs. 10-11.

12     *Non-Darcy Flow:* In case of high **Forchheimer number ( $F_{oc}>0.11$ )** in the hydraulic fractures, the  
 13    linear Darcy flow is no longer applicable (Zeng and Grigg, 2006). The permeability correction factor  
 14    (Barree and Conway, 2004) for Darcy-Forchheimer flow can be expressed as follows:

15                          
$$F_{app} = \frac{2}{1 + \sqrt{1 + 4\rho_g \beta \left( \frac{k_0}{\mu_g} \right)^2 |\nabla p|}} \quad (12)$$



16     **Fig. 6 – Permeability correction factor  $F_{app}$  versus Knudsen number for all flow regions with**

methane properties in Table 2,  $T=191$  K,  $k_0=1\text{e-}10$  and  $\phi=0.1$

where  $\beta$  is the empirical Forchheimer coefficient, for propped hydraulic fractures, which can be evaluated as follows (Rubin, 2010):

$$\beta = 3.2808 \frac{1.485 \times 10^9}{(k_0 \times 10^{-15})^{1.021}} \quad (13)$$

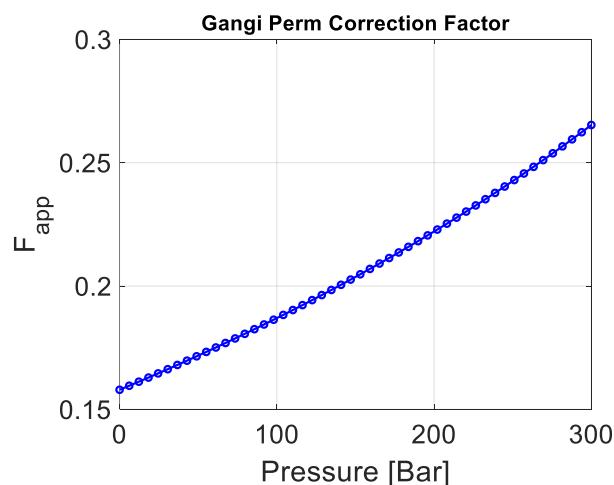
## 2.3 Geomechanics effect

As shown in Fig. 2, shale reservoir has multi-scale fractures. The fracture conductivity will be decreased with increasing of production time due to the proppant embedment and fracture closure under high stress concentration near the fracture (Akkutlu et al, 2018, Hu et al, 2018a, 2018b). In this paper, three types of fractures are defined based on their various length scales, including hydraulic fracture (half-length 50-100 meters, aperture 1mm), natural fracture (half-length 1-20 m, aperture 0.1mm), and micro-fracture (half-length < 1m, aperture <0.1 mm). A new geomechanics model is proposed herein by considering closure of micro-fracture, unpropped natural fracture and propped fractures.

To consider the micro-fracture closure, Gangi's (1978) empirical pressure-dependent permeability reduction model can be applied as follows:

$$k = k_0 F_{app} = k_0 \left[ 1 - \left( \frac{P_c - \alpha_B p}{P_1} \right)^m \right]^3 \quad (14)$$

Where  $\alpha_B$  is the Biot's constant,  $P_c$  is the confining overburden pressure,  $P_I$  is the effective stress when micro-fracture completely closed.  $m$  is a constant related to surface roughness. **Fig. 7** shows an estimation of Gangi permeability correction factor for methane using Eqs. 14.



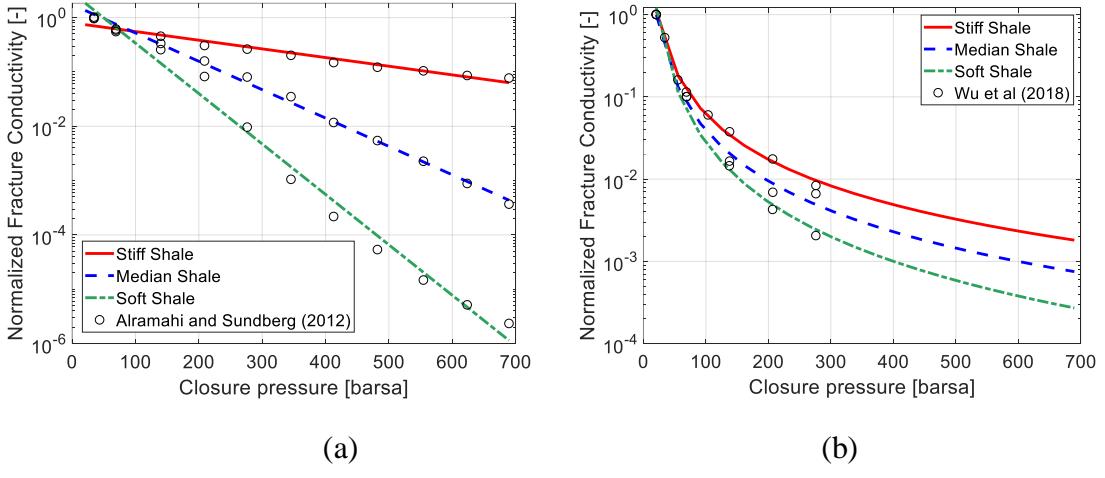
1           **Fig. 7 – Permeability correction factor  $F_{\text{frac}}$  versus pore pressure with  $m=0.5$ ,  $p_1=180$  MPa,  
2            $p_c=38$  MPa and  $\alpha=0.5$**

3           To consider the closure of hydraulic and natural fractures, Alramahi and Sundberg (2012)  
4           performed experiment to measure the effect of closure pressure on propped fracture conductivity for  
5           different shale samples from stiff shale to soft shale. An empirical model of normalized fracture  
6           conductivity for propped fractures,  $F_{cd,N}$ , can be fitted as follows:

$$\begin{aligned} \text{Stiff Shale: } F_{cd,N}(p) &= 10^{-0.00011\sigma - 0.0971}, \quad R^2 = 0.961 \\ \text{Medium Shale: } F_{cd,N}(p) &= 10^{-0.00035\sigma + 0.2396}, \quad R^2 = 0.996 \\ \text{Soft Shale: } F_{cd,N}(p) &= 10^{-0.00064\sigma - 0.4585}, \quad R^2 = 0.987 \end{aligned} \quad (15)$$

8           Wu et al (2018) performed similar experiment to investigate the effect of closure pressure on  
9           unpropped fracture conductivity. An empirical model of normalized fracture conductivity for  
10          unpropped fractures can be fitted as follows:

$$\begin{aligned} \text{Stiff Shale: } F_{cd,N}(p) &= 10^{-0.793\ln(\sigma_c) + 4.5618}, \quad R^2 = 0.995 \\ \text{Medium Shale: } F_{cd,N}(p) &= 10^{-0.89\ln(\sigma_c) + 5.0725}, \quad R^2 = 0.988 \\ \text{Soft Shale: } F_{cd,N}(p) &= 10^{-1.041\ln(\sigma_c) + 6.0216}, \quad R^2 = 0.989 \end{aligned} \quad (16)$$



14           **Fig. 8 – Empirical correlation between normalized fracture conductivity and closure  
15          pressure for propped fractures (a) and unpropped fractures (b)**

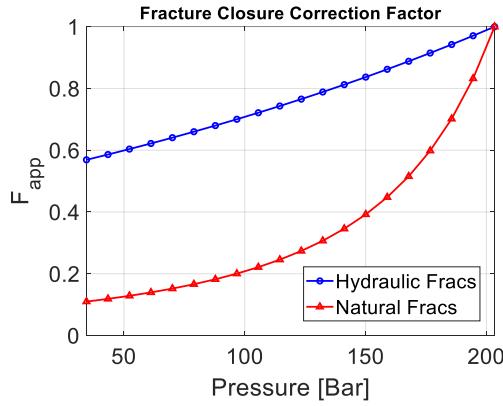
16           Where effective closure stress  $\sigma_c$  can be calculated by reservoir horizontal stress and in-situ  
17          fracture pore pressure,  $\sigma_c(p) = \sigma_h - p$ . Plane direction of hydraulic fracture is normally orthogonal  
18          to the minimum horizontal stress and it support by rigid proppant, while the plane of natural fracture  
19          has stochastic orientation and lacking support from proppant. Thus, the closure stress for hydraulic  
20          fracture and natural fracture can be expressed as follows:

$$\begin{aligned}
1 & \text{ HydraulicFrac: } \sigma_{HF} = \sigma_{h\min} - p \\
2 & \text{ NaturalFrac: } \sigma_{NF} = \frac{\sigma_{h\min} + \sigma_{h\max}}{2} - p
\end{aligned} \tag{17}$$

2 The empirical correlation between fracture conductivity and closure pressure are shown in **Fig.**  
3 **8.** In the OpenShale, the fracture permeability can be reduced by a dynamic permeability correction  
4 factor as follows:

$$5 \quad k_f = k_0 F_{app} = k_0 \frac{F_{cd}(p)}{F_{cd}(p_0)} \tag{18}$$

6 Based on proposed empirical correlation model in Eqs. 15-16, a typical permeability correction  
7 factors for fracture closure can be shown as follows (**Fig. 9**):



8 **Fig 9 – Permeability correction factor F<sub>frac</sub> for hydraulic fractures and natural fractures**  
9 with  $p_o = 20.34 \text{ MPa}$  and  $p_{wf} = 34.5 \text{ MPa}$   $\sigma_{h\min} = 29 \text{ MPa}$  and  $\sigma_{h\max} = 34 \text{ MPa}$

### 11 3 Numerical Model

12 In this paper, a new shale gas simulation framework, OpenShale , is developed using the automatic  
13 differentiation module (ad-core, ad-props), black-oil module (ad-blackoil) and hierarchical fracture  
14 model (hfm) module in open-source MATLAB Reservoir Simulation Toolbox (Lie, 2012). Two-point  
15 flux approximated finite volume method (TPFA-FVM) is applied for discretizing the governing  
16 equations (Eq. 3). Time discretization is implemented using a fully implicit first-order backward  
17 scheme, where the Jacobian matrix of the nonlinear system is calculated by Automatic  
18 Differentiation. All nonlinear functions for shale gas transport and storage mechanisms as well as  
19 geomechanics effect are defined as separate function. For multi-scale fracture system, the larger  
20 fracture, such as the hydraulic fracture and natural fracture are explicitly modeled using EDFM. The  
21 micro-fractures are assumed highly connected and thus upscaled into the matrix permeability.

1           **3.1 Numerical discretization**

2           The discretized governing equation of Eq. 3 can be expressed as follows:

$$\begin{aligned}
 & \frac{\phi V}{\Delta t} (b_g(p^{n+1}) - b_g(p^n)) + \frac{(1-\phi)V}{\Delta t} \frac{1}{\rho_{gsc}} (m_{ad}(p^{n+1}) - m_{ad}(p^n)) \\
 & - \mathbf{div} \left( b_g(p^{n+1}) \frac{\prod_i F_{app,i}(p^{n+1})}{\mu_g(p^{n+1})} T \cdot \mathbf{grad}(p^{n+1}) \right) \\
 & - V b_g(p^{n+1}) q_w(p^{n+1}) - V b_g(p^{n+1}) \psi_{f-m}(p^{n+1}) = 0
 \end{aligned} \tag{19}$$

4           The discretized governing equation for each 1D fracture system can be expressed as follows:

$$\begin{aligned}
 & \frac{\phi V}{\Delta t} (b_g(p^{n+1}) - b_g(p^n)) \\
 & - \mathbf{div} \left( b_g(p^{n+1}) \frac{\prod_i F_{app,i}(p^{n+1})}{\mu_g(p^{n+1})} T \cdot \mathbf{grad}(p^{n+1}) \right) \\
 & - V b_g(p^{n+1}) q_w(p^{n+1}) - V b_g(p^{n+1}) \psi_{m-f}(p^{n+1}) = 0
 \end{aligned} \tag{20}$$

5           where  $V$  is the bulk volume of a grid cell.  $\psi_{f-m/m-f}$  is the flow coupling term between fracture  
6           and matrix. To simplify the implementation of governing equations (Eqs. 18-19), three discrete  
7           domain delta  $\delta$  functions for matrix ( $\Omega_m$ ), hydraulic fractures ( $\Omega_{HF}$ ) and natural fractures ( $\Omega_{NF}$ ) can  
8           be defined as follows:

$$\delta_m(x) = \begin{cases} 1 & x \in \Omega_m \\ 0 & x \notin \Omega_m \end{cases}, \quad \delta_{HF}(x) = \begin{cases} 1 & x \in \Omega_{HF} \\ 0 & x \notin \Omega_{HF} \end{cases}, \quad \delta_{NF}(x) = \begin{cases} 1 & x \in \Omega_{NF} \\ 0 & x \notin \Omega_{NF} \end{cases} \tag{21}$$

10           A generic numerical model for fractured reservoir considering shale gas transport and storage  
11           mechanism can be expressed as follows:

$$\begin{aligned}
 & \frac{\phi V_{ijk}}{\Delta t} (b_g(p^{n+1}) - b_g(p^n)) + \delta_m \frac{(1-\phi)V_{ijk}}{\Delta t} \frac{1}{\rho_{gsc}} (m_{ad}(p^{n+1}) - m_{ad}(p^n)) \\
 & - \mathbf{div} \left( b_g(p^{n+1}) \frac{\prod_i [1 + \delta_{HF/NF,i} F_{app,i}(p^{n+1})]}{\mu_g(p^{n+1})} T \cdot \mathbf{grad}(p^{n+1}) \right) \\
 & - V_{ijk} b_g(p^{n+1}) q_w(p^{n+1}) - V_{ijk} b_g(p^{n+1}) \psi_{f-m/m-f}(p^{n+1}) = 0
 \end{aligned} \tag{22}$$

14           Assuming vertical well fully penetrate the reservoir thickness, a semi-analytical well model  
15           (Peaceman, 1983) for a vertical well can be expressed as follows:

$$q_w = WI / \mu_g (p_{bh} - p) \tag{23}$$

1 where  $p_{bh}$  is the bottom hole pressure of a wellbore, M/L/T<sup>2</sup>. WI is the wellbore flow index.

2 The solution matrix from Eqs. 21 can be expressed as follows:

3

$$\begin{bmatrix} \mathbf{A}_{mm} & \mathbf{A}_{mf} & \mathbf{A}_{mw} \\ \mathbf{A}_{fm} & \mathbf{A}_{ff} & \mathbf{A}_{fw} \\ \mathbf{A}_{wm} & \mathbf{A}_{wf} & \mathbf{A}_{ww} \end{bmatrix} \begin{Bmatrix} \mathbf{p}_m \\ \mathbf{p}_f \\ \mathbf{p}_w \end{Bmatrix} = \begin{Bmatrix} \mathbf{Q}_m \\ \mathbf{Q}_f \\ \mathbf{Q}_w \end{Bmatrix} \quad (24)$$

#  $\mathbf{p}_m$  = # MatrixEles, #  $\mathbf{p}_f$  = # FractureEles, #  $\mathbf{p}_w$  = #Eles has well

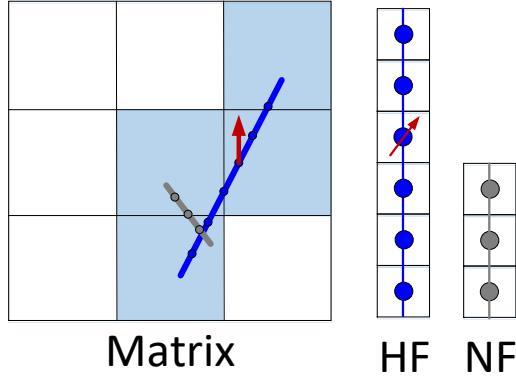
4 Noted that the shale gas viscosity, density and permeability corrections terms are all depends on  
5 solution variables. To solve non-linear system of Eq. 23, the residual form of Newton's iterations can  
6 be expressed as follows:

7

$$\mathbf{J}(\mathbf{x}^i)(\mathbf{x}^{i+1} - \mathbf{x}^i) = \frac{d\mathbf{R}}{d\mathbf{x}}(\mathbf{x}^i)(\mathbf{x}^{i+1} - \mathbf{x}^i) = -\mathbf{R}(\mathbf{x}^i) \quad (25)$$

8 The Jacobian matrix  $\mathbf{J}$  is calculated by automatic differentiation in MRST.

9 **3.2 EDFM**

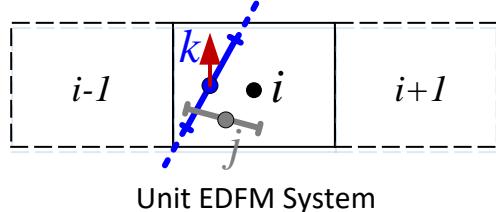


10 **Fig. 10 – Grid system in EDFM for matrix, natural fracture and hydraulic fracture**

11 As shown in **Fig. 10**, EDFM adopted the concept of dual-continuum fracture modeling method,  
12 the flow coupling term  $\psi_{f-m/m-f}$  is introduced to couple the solution among matrix and fractures.  
13 Thus, the matrix grid is not necessary conforming with the fracture plane. As shown in **Fig. 11**, there  
14 are three kinds of non-neighbor connection (NNC) in EDFM formulation: 1) fracture-matrix  
15 connectivity, 2) fracture-fracture connectivity and 3) fracture-well connectivity. The general NNC  
16 model can be expressed as follows (Xu, 2015):

17

$$\begin{aligned} \psi_{f-m}^{NNC} &= T_{f-m}^{NNC}(p_f^{n+1} - p_m^{n+1}) \\ \psi_{f-m}^{NNC} &= -\psi_{m-f}^{NNC} \end{aligned} \quad (26)$$



**Fig. 11 – Unit EDFM NNCs of 1) fracture-matrix ( $i$ - $k$  pair) connectivity 2) fracture-fracture ( $j$ - $k$  pair) connectivity and 3) fracture-wellbore (well- $k$  pair) connectivity**

*Fracture-matrix NNC:* The fracture-matrix transmissibility ( $T_{f-m}$ ) can be expressed as follows:

$$T_{ik}^{NNC} = \frac{k_{0,ik}}{\mu_{g,ik}} \frac{A_{ik}}{\langle d \rangle_{ik}} \quad (27)$$

where  $A_{i,k}$  is the intersection area fraction between a fracture plane and a gridblock. For 2D grid, the area is the product of intersected fracture cell length within the matrix cell and uniform formation thickness,  $DZ$ . Noted that the harmonic average and upwind scheme are used for the permeability and viscosity, respectively.  $\langle d \rangle_{i,k}$  is the average normal distance between matrix cell and fracture plane, which can be calculated as follows:

$$\langle d \rangle_{ik} = \frac{\int d_{ik} dv}{V_i} \quad (28)$$

For 2D structured grid, an analytical solution is available for the average normal distance (see Tene et al, 2016).

*Fracture-fracture NNC:* the star-delta transformation can be used to calculate the transmissibility between intersected fractures as follows (Hajibeygi et al, 2011):

$$T_{jk}^{NNC} = \frac{t_j t_k}{\sum_{m=1}^{N_{ints}} t_m}, \quad t_m = \frac{A_{f,m}}{0.5 h_{f,m}} \frac{k_{0,m}}{\mu_{g,m}} \quad (29)$$

where  $A_f$  is the cross-section area of a fracture plane, for 2D cell, which can be calculated by product of fracture aperture,  $w_f$ , and formation thickness.  $h_f$  is the fracture cell length.

*Fracture-well NNC:* If a well intersected with a fracture cell, the effective wellbore index (WI) and equivalent radius ( $r_e$ ) can be expressed as follows (Xu, 2015):

$$WI_f = \frac{2\pi k_f w_f}{\ln(r_e / r_w) + s}, \quad r_e = 0.14 \sqrt{h_f^2 + DZ^2} \quad (30)$$

1 where  $s$  is the skin factor, dimensionless, which will be used as a correction factor to correct the  
 2 error introduced by EDFM when model low-permeability fractures.  $DZ$  is the formation thickness,  $L$ .

## 3 **4 Verification**

4 To verify the presented general shale gas model (Eq. 21), two numerical simulations are  
 5 performed against a commercial simulator (CMG, 2015) and an in-house simulator with unstructured  
 6 mesh (Jiang and Younis, 2015). The base model and simulation parameters for all cases as shown in  
 7 **Table 3:**

8 **Table 3—Base model and simulation parameters for all cases**

Property	Unit	Value
Rock density	kg/m <sup>3</sup>	2500
Molecular weight, CH <sub>4</sub>	kg/mol	0.01604
Critical pressure, CH <sub>4</sub>	MPa	4.60
Critical temperature, CH <sub>4</sub>	K	190.6
Acentric factor, CH <sub>4</sub>	-	0.01142
Well radius	m	0.1

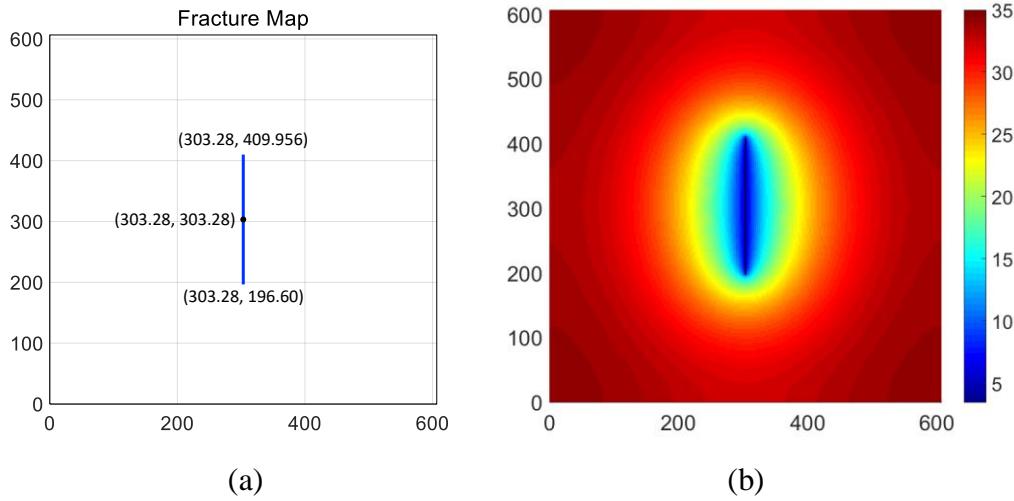
### 9 **4.1 Case 1 – Verification against commercial simulator**

10 OpenShale is firstly verified in a simple methane production case against a commercial  
 11 simulator (CMG) with a single vertical hydraulic fracture (**Fig. 12**). By changing the hydraulic  
 12 conductivity, grid schemes and natural fractures, three subcases (Case1a, Case1b and Case1c) are  
 13 investigated. The accuracy of OpenShale with explicit fracture modeling (EFM) and EDFM are  
 14 systematically studied. In this simulation, only Langmuir adsorption (Eq. 8) is considered. All fluid  
 15 properties and simulation parameters are the same with the commercial simulator. The  
 16 compressibility factor Z and natural gas viscosity are directly interpolated from the properties table  
 17 of the commercial simulator. Detailed simulation properties are shown in **Table 4**.

18 **Table 4. Key reservoir and simulation parameters of Case 1**

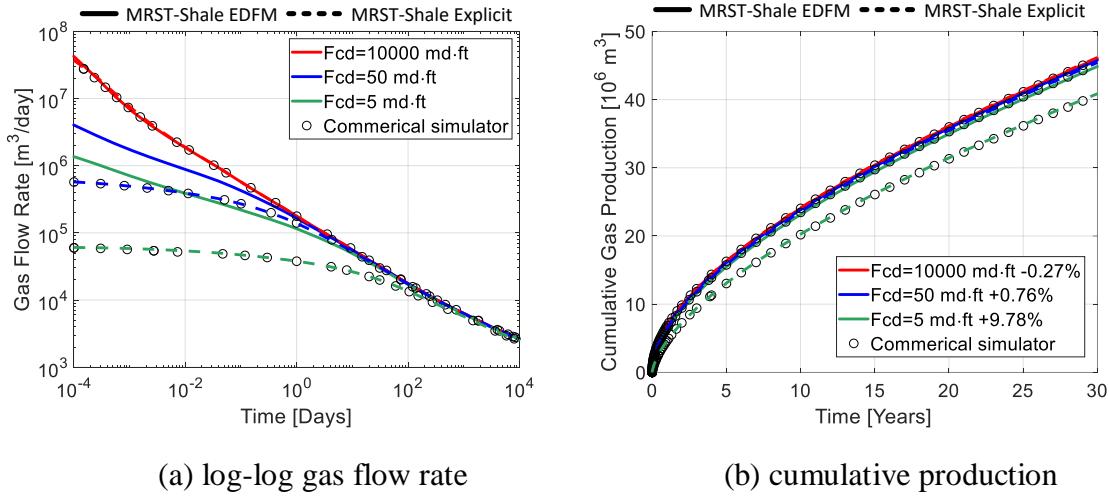
Property	Unit	Value
Domain dimensions (x,y)	m	606.6,606.6
Grid (nx,ny)	-	201,65
Formation thickness	m	45.72
Initial reservoir pressure	MPa	34.47
Temperature	K	327.60
Langmuir pressure	MPa	8.96
Langmuir volume	m <sup>3</sup> /kg	0.0041
Matrix porosity		0.07

Matrix compressibility	1/Pa	1.45e-10
Matrix permeability	nD	500
Fracture permeability	mD	0.5-1000
Fracture width	m	0.003
Fracture half-length	m	106.68
Fracture conductivity	md-ft	5-10000
Well BHP	MPa	3.45
Production time	years	30



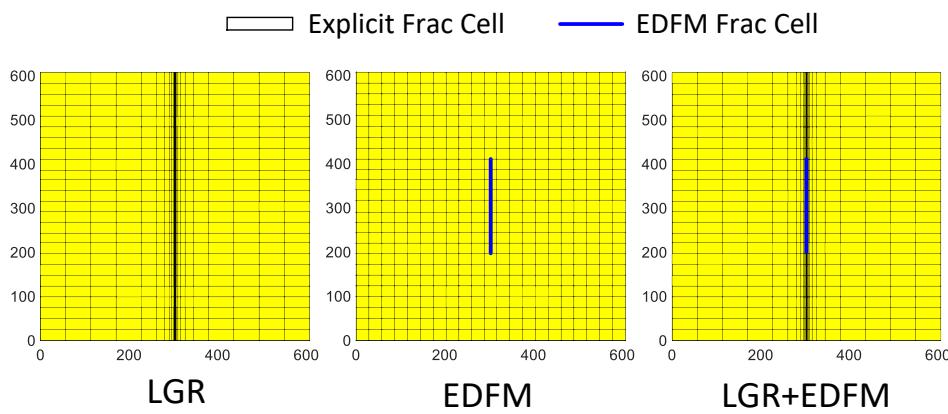
**Fig. 12 Fracture map (a) and pressure contour after 30 years production (b) of Case 1a and Case1b**

*Case1a:* In the first subcase, three fracture conductivities (10000 md-ft, 50 md-ft, 5 md-ft) are used to verify the accuracy of OpenShale with EFM and EDFM. **Fig. 13** shows a good agreement of both gas flow rate and cumulative production between OpenShale and commercial simulator. Results show that OpenShale with EFM (dash line) always gives consistent results against commercial simulator. But OpenShale with EDFM (solid) has significant error (up to 10.92%) when fracture conductivity is low (5 md-ft). Fig. 12a shows that OpenShale EDFM only converges to reference solution under infinite fracture conductivity (10000 md-ft). This is observation matches Tene (2017)'s conclusion that EDFM can not handle the fracture with low permeability.



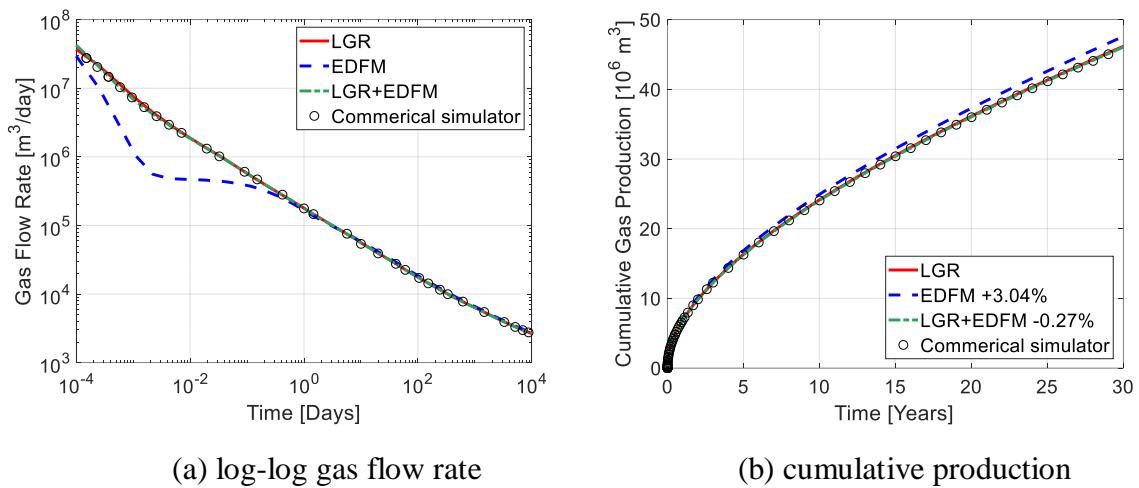
**Fig. 13 Comparison of gas flow rate (a) and cumulative production (b) for Case 1a between OpenShale EDFM (solid line), OpenShale EFM (dash line) and a commercial simulator (dots) with respect to fracture conductivities of 5 md-ft (green lines), 50 md-ft (blue lines) and 10000 md-ft (red lines)**

**Case1b:** For unconventional tight reservoir, LGR is usually required to capture the transient flow behavior and sharp pressure gradient near the hydraulic fractures. In the second subcase, the effect of grid schemes on accuracy of OpenShale with EFM and EDFM are investigated. In this case, the fracture conductivity is set as 10000 md-ft to eliminate the EDFM error mentioned in Case1a. All other parameter is the same with Case1a. As shown in Fig. 14, three grid schemes are investigated, where LGR scheme with logarithmic refinement that is solved by OpenShale EFM; EDFM scheme is the standard EDFM grid scheme (Xu et al, 2017 and Tene et al, 2017) with uniform grid that is solved by EDFM; EDFM+LGR scheme is the same grid scheme as LGR scheme that an additional EDFM fracture cell is added and that is solved by EDFM. Noted that all grid scheme has the same grid dimension ( $nx, ny$ ) of 499x61.



1           **Fig. 14 EFM and EDFM Grid schemes for Case1b, fracture cell is shown 10 times larger**  
 2       **than the real size, where logarithmic refinement and uniform used in LGR and EDFM scheme,**  
 3       **respectively**

4       **Figs. 15-16** shows a good agreement of gas flow rate and cumulative production between  
 5       OpenShale and commercial simulator with respect to high fracture conductivity and low fracture  
 6       conductivity. OpenShale with EFM again gives consistent results against commercial simulator for  
 7       all grid schemes. However, the standard EDFM grid scheme can introduce an error of 3.31% for high  
 8       fracture conductivity and 1.11% for low fracture conductivity. The error is measured by the  
 9       difference of cumulative production between grid schemes of LGR+EDFM and EDFM. This  
 10      benchmark case demonstrates that EDFM cannot capture transient flow behavior and sharp pressure  
 11      gradient near the hydraulic fracture without helping of LGR.



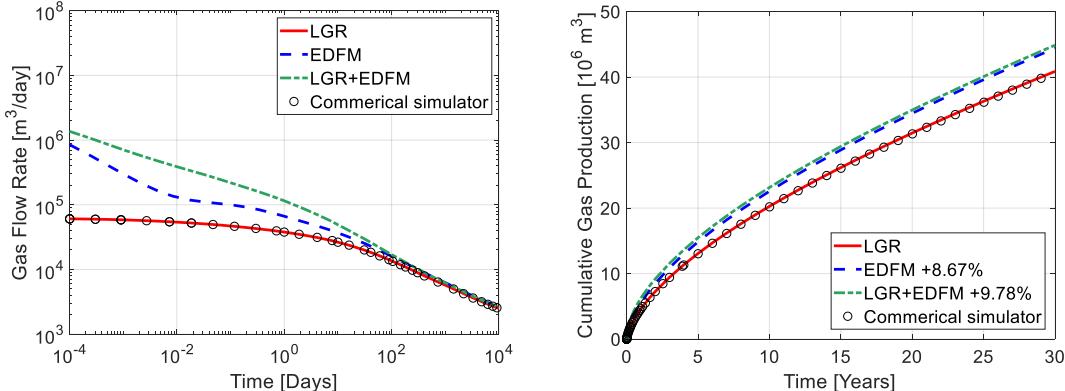
12           (a) log-log gas flow rate

13           (b) cumulative production

14           **Fig. 15 Comparison of gas flow rate (a) and cumulative production (b) for Case 1b with**

15       **high fracture conductivity of 10000 md-ft between OpenShale and a commercial simulator**

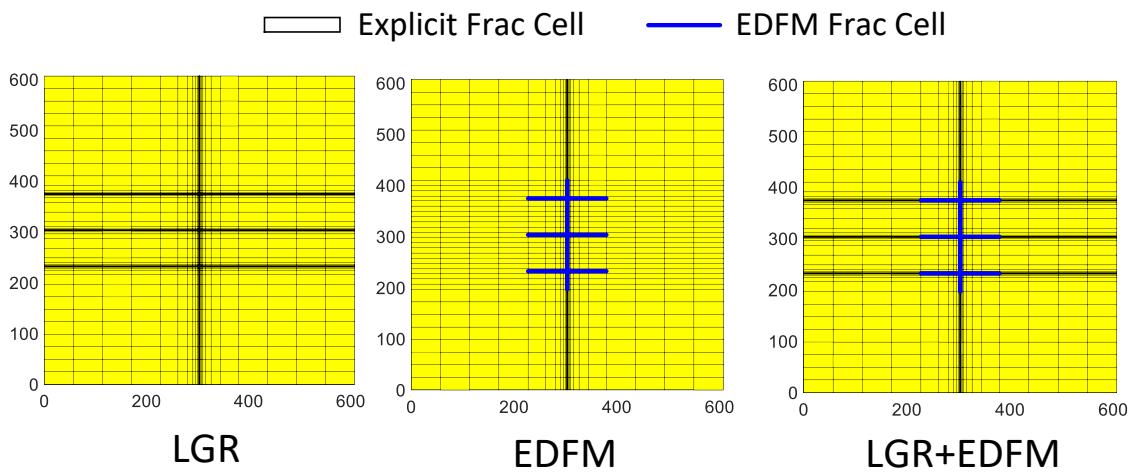
16           (dots)





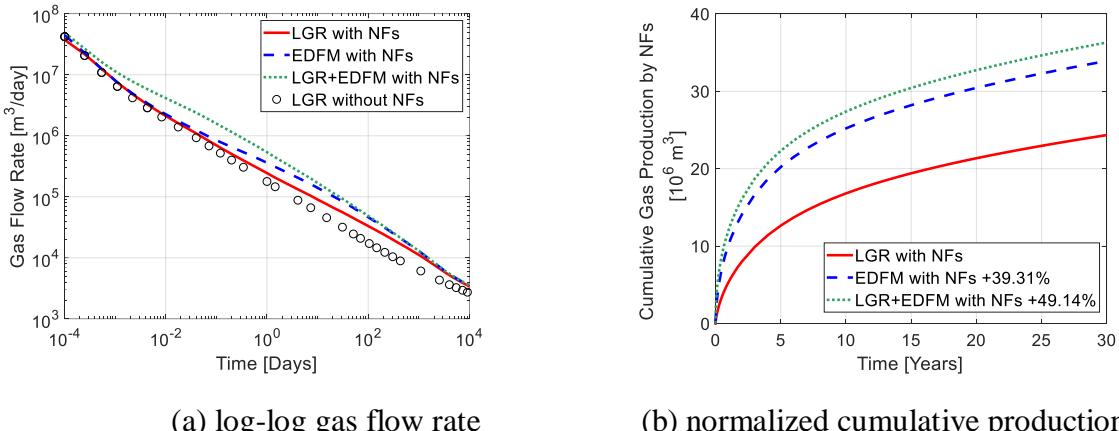
**Fig. 16 Comparison of gas flow rate (a) and cumulative production (b) for Case 1b with fracture conductivity of 5 md-ft between OpenShale and a commercial simulator (dots)**

**Case1c:** As mentioned in Case1a and Case1b, EDFM cannot handle low-permeability fracture and hydraulic fractures with sharp pressure gradient. But modeling of natural fracture network is quite challenge for the EFM. In this subcase, the effect of different grid schemes of natural fractures on accuracy for OpenShale with EDFM is also investigated. As shown in Fig. 17, six natural fractures with the same length of 116.74 m are added based on the Case1a. The well performance of two grid schemes with and without LGR for natural fractures are studied. Fracture conductivity for hydraulic fracture and natural fractures are set as 10000 md-ft and 5 md-ft, respectively. All other parameters are the same with Table 3.



**Fig. 17 Grid schemes of Case 1c, number of grids are shown 20 times coarser than the real one. LGR scheme with LGR for natural fractures, EDFM scheme without LGR for natural fractures**

**Fig. 18** demonstrates that OpenShale with EDFM can lead to a significant error (up to 16.99%) for the case where low-permeability natural fractures connected with high-permeability hydraulic fractures. Also, EDFM without LGR for natural fractures tends to underestimate the well performance (error of 3.4% for six natural fractures). This benchmark case indicates that EDFM is not capable to accurately model well performance of shale gas flow in ultra-tight reservoir due to the errors introduced by low-permeability fracture and grid refinement.

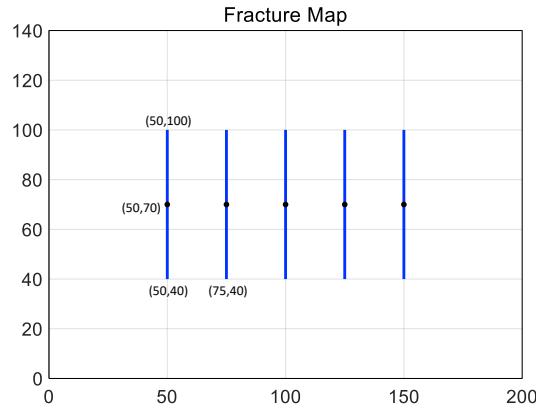


**Fig. 18 Comparison of gas flow rate (a) and normalized cumulative production by NFs (b) for Case 1c between different grid scheme for natural fractures**

In sum, this case study shows that OpenShale with EFM always give consistence results against commercial simulator, while OpenShale with EDFM only converge to the reference solution at infinite fracture conductivity (Case1a). Also, OpenShale with EDFM cannot handle low-permeability fracture (Case1b) and cannot capture transient behavior and sharp gradient without LGR (Case1c). OpenShale with EDFM can model complex and irregular natural fractures accurately and efficiently. Thus, in the following simulations, an empirical skin-factor and uniform grid refinement are adopted to relieve the limitations of EDFM. More advanced projected EDFM (Tene et al, 2017) and adaptively grid refinement will be implemented in our future work.

#### 4.2 Case 2 – Verification against in-house simulator

OpenShale is further verified against an in-house simulator (Jiang and Younis, 2015) by considering more comprehensive state-of-art transport mechanisms and fracture geometries. For the reference solution, it used fully unstructured mesh with LGR to capture the complex fracture geometries as well as the sharp pressure gradient near the fracture. In this case, the gas rate solution of two sub-case are investigated. In the first sub-case (Case2a), the well performance with and without storage (Eq. 8) and transport mechanism (Eq. 10) is considered. In the second sub-case (Case2b), the irregular fracture geometry is considered. The fracture map of Case2a is shown in **Fig. 19**. Detailed simulation parameters for Case 2 are elaborated in **Table 4**.



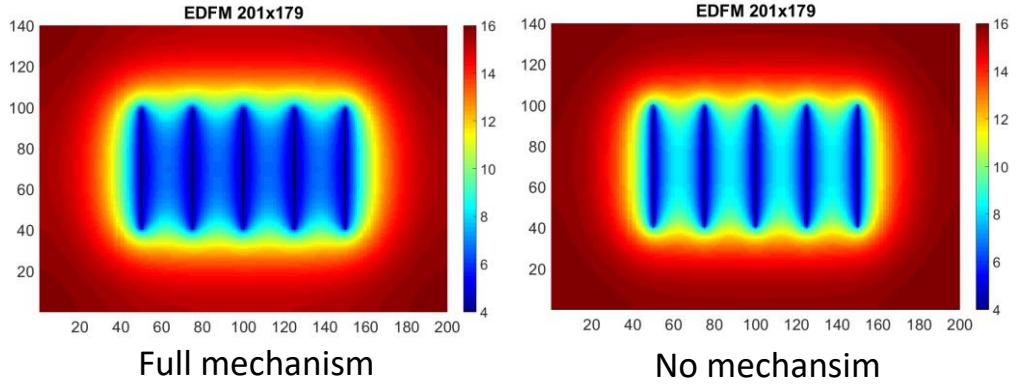
**Fig. 19 Fracture map and EDFM grid of Case 2**

**Table 4. Key reservoir and simulation parameters of Case 2**

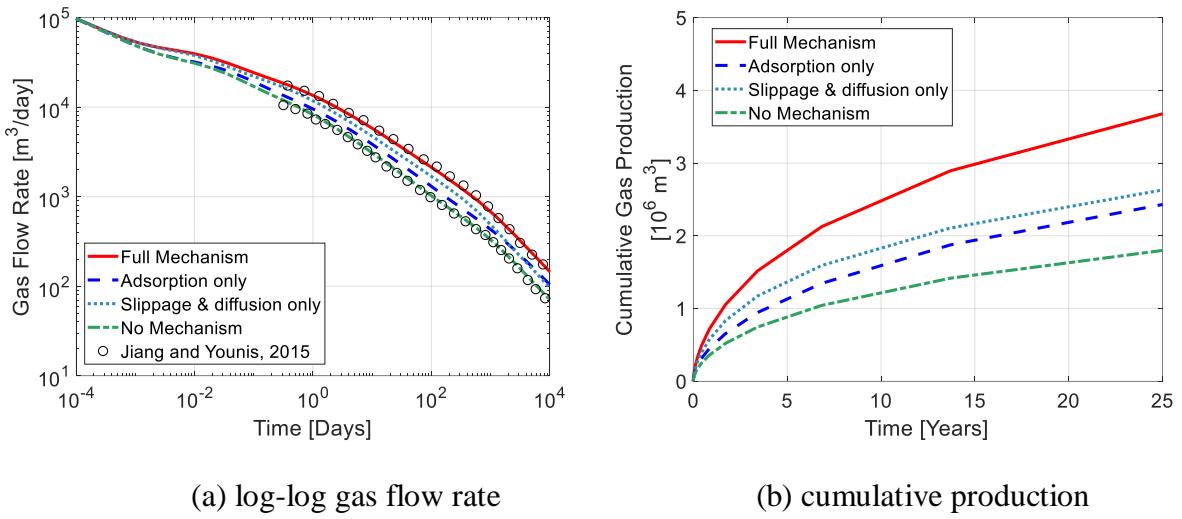
Property	Unit	Value
Domain dimensions (x,y)	m	200,140
Formation thickness,	m	10
Initial reservoir pressure	MPa	16
Temperature	K	343.15
Langmuir pressure	MPa	4
Langmuir volume	$\text{m}^3/\text{kg}$	0.018
Matrix porosity		0.1
Matrix compressibility	1/Pa	1.0e-9
Fracture porosity		1.0
Matrix permeability	nD	100
Fracture permeability	D	1
Fracture width	m	1e-3
Well BHP	MPa	4
Correction skin factor	-	43
Production time	days	10000

Other parameters are the same as in Table 2

**Fig. 20** shows pressure contour after 2500 days of production for Case 2 with and without transport mechanisms. It can be observed that the sub-case with full mechanism has better pressure depletion (dark blue region) than one without any mechanism. **Fig. 21** shows a good agreement between gas flow rate between OpenShale and an in-house simulator, where demonstrates that the both adsorption and gas slippage and diffusion effect increase the gas production significantly. In tight unconventional reservoirs, smaller pore-throat and lower bottom-hole pressure can lead to higher production due to gas slippage flow and releasing adsorbed gas.



**Fig. 20 Pressure contour with and without full shale gas transport mechanism @ 2500 days of Case 2**



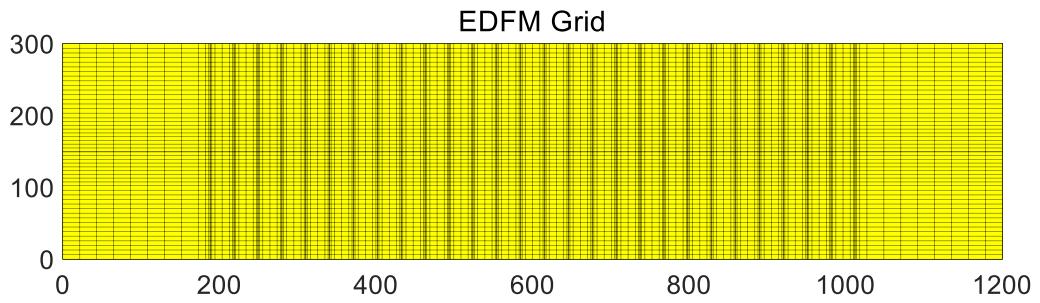
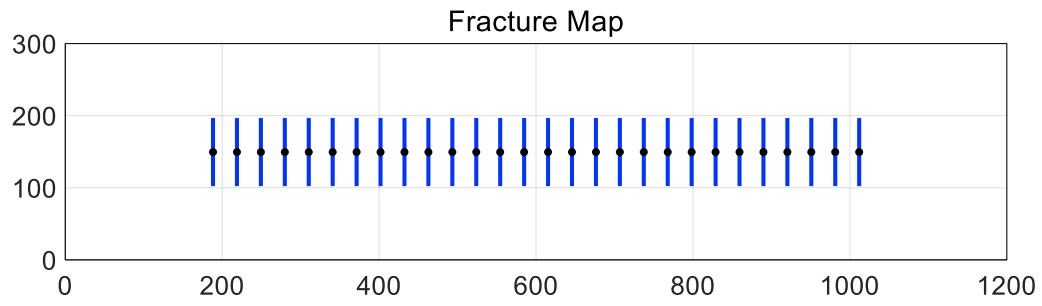
**Fig. 21 Comparison of gas flow rate (a) and cumulative production (b) for Case 2a between OpenShale and an in-house simulator**

## 5 Application

In the previous sections, OpenShale shows its capability to handle arbitrary transport and storage mechanism and fracture geometries. To further illustrate the applicability of OpenShale in practical problems, two case studies of OpenShale in realistic unconventional reservoirs with complex fracture network are presented.

### 5.1 Case 3: History matching and production forecast

To further verify the applicability of the OpenShale. A history matching with field production data on a Barnett shale has performed. The field production and simulation data are adopted from literature (Cao, Liu and Leong, 2016; Yu and Kamy Sepehrnoori, 2014). The detailed reservoir and fluid parameters are shown as in **Fig. 22** and **Table 5**.



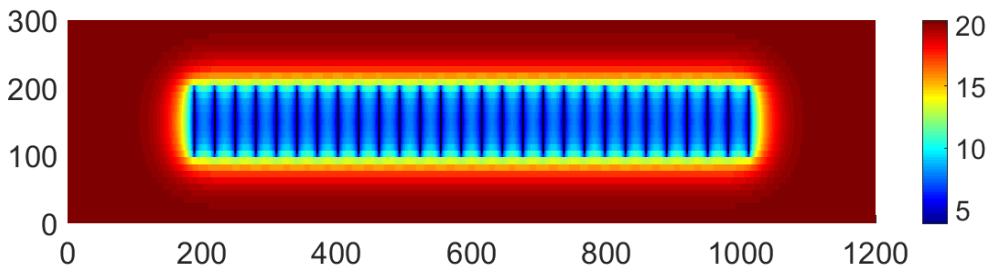
**Fig. 22 Fracture map and EDFM LGR grid with 28 planar hydraulic fractures of Case 3**

**Table 5. Key reservoir and simulation parameters of Barnett shale for Case 3 (Cao, 2016)**

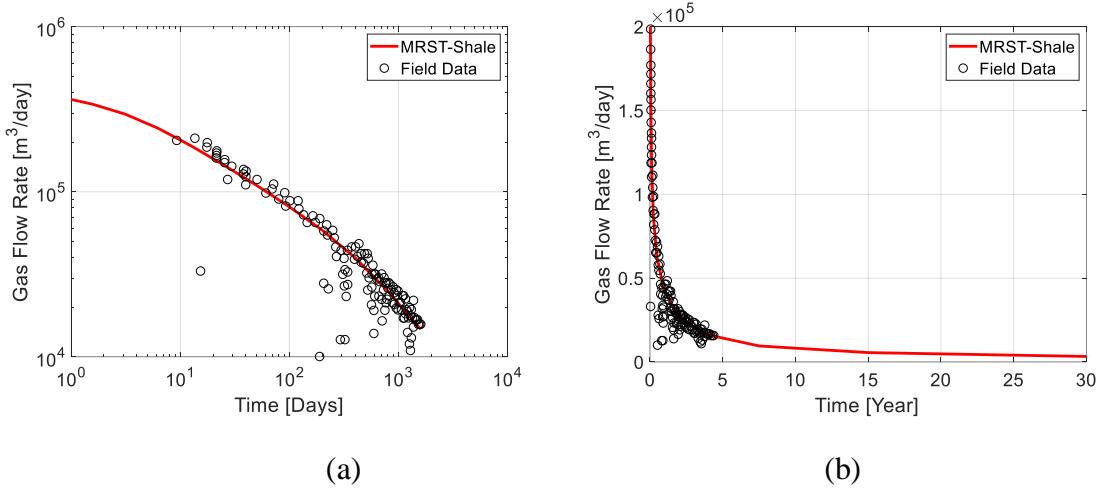
Property	Unit	Value
Domain dimensions (x,y)	m	1200,300
Depth	m	5463
Formation thickness,	m	90
Initial reservoir pressure	MPa	20.34
Temperature	K	352
Rock density	kg/m <sup>3</sup>	2500
Langmuir pressure	MPa	4.47
Langmuir volume	m <sup>3</sup> /kg	0.00272
Matrix porosity		0.03
Matrix compressibility	1/Pa	1.5e-10
Fracture compressibility	1/Pa	1.0e-8
Matrix permeability	nD	200
Fracture permeability	mD	100
Fracture width	m	0.003
Fracture spacing	m	30.5
Fracture half-length	m	47.2
Fracture conductivity	md-ft	1
Well BHP	MPa	3.69
Correction skin factor	-	19
Production time	days	1600

Other parameters are the same as in Table 2

1 In this simulation, a rectangle reservoir with dimension of  $1100 \times 290 \times 90$  m was discretized  
 2 by  $148 \times 39 \times 1$  grids. 28 stages hydraulic fractures in the center of domain with the half-length of  
 3 47.2 m and the fracture spacing of 30.5 m. The fractures are assumed have constant aperture of 0.003  
 4 m and permeability of 100 md. Only shale gas storage mechanism of Langmuir adsorption (Eq. 8) is  
 5 considered. **Fig. 23** shows the pressure contour at different production time (400 days and 1600  
 6 days). **Fig. 24** shows the comparison of production rate between OpenShale and field data which  
 7 shows good agreements with the field production data. Based on matched simulation parameters, the  
 8 production forecast can be easily performed as in Fig. 21.

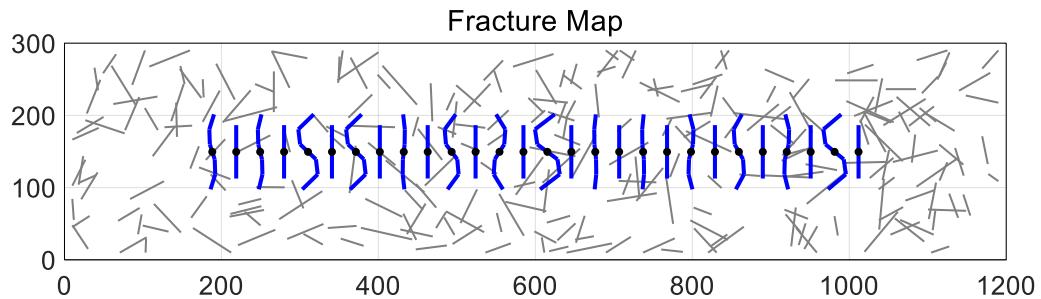


9  
 10 **Figure 23 Pressure contour after 1600 days production for Barnett shale reservoir (Case 3)**



11  
 12 **Fig. 24 History matching (a) and production forecast (b) of a Barnett shale well (Case 3)**  
 13  
 14 **5.2 Case 4: New model evaluation**

15 To illustrate the capability of modular design and rapid prototyping of OpenShale, a new shale  
 16 gas model considering geomechanics effect (Eqs. 15-17) for multi-scale fractured network is  
 17 implemented and evaluated using OpenShale. In this section, the influence of multi-scale fracture  
 18 network and geomechanics effect on shale gas production performance will be investigated.



**Fig. 25 Fracture map with 28 non-planar hydraulic fractures and 248 natural fractures of Case 4**

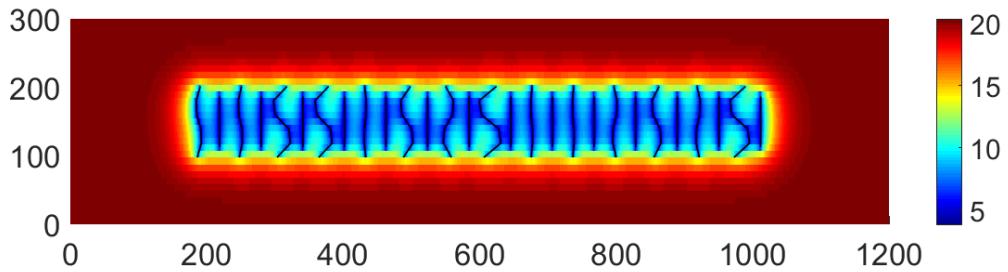
In this case, all the simulation parameters are the same with Case 3 of Barnett shale reservoir.

The total length of non-planar hydraulic fractures (blue lines in **Fig. 25**) is the same as planar fractures used in Case 3 (blue lines in Fig. 14). Natural fractures are stochastically generated by an open-source fracture generator ADFNE (Alghalandis, 2017). The geomechanics parameters for shale reservoir are assumed (Wasaki and Akkutlu, 2015) as follows (**Table 5**):

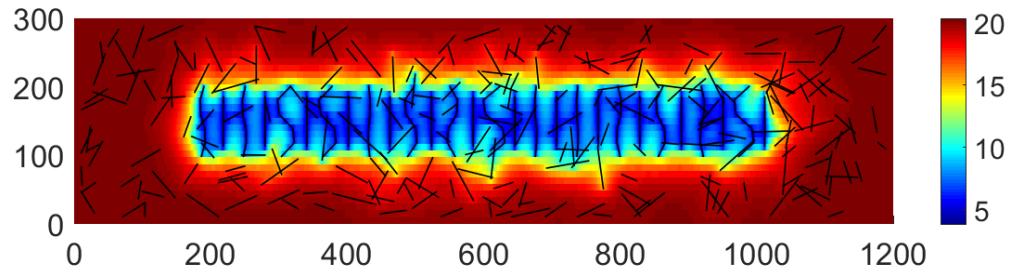
**Table 5. Geomechanics parameters of Barnet shale for Case 4**

Property	Unit	Value
Biot constant, $\alpha$	-	0.5
Overburden confining stress, $p_c$	MPa	38
Maximum horizontal stress, $s_{hmax}$	MPa	34
Minimum horizontal stress, $s_{hmin}$	MPa	29
Maximum closure stress for micro-fracture, $p_l$	MPa	180
Gangi exponential constant, $m$	-	0.5
Natural fractures permeability	md	10

Other parameters are the same as in Tables 2-3

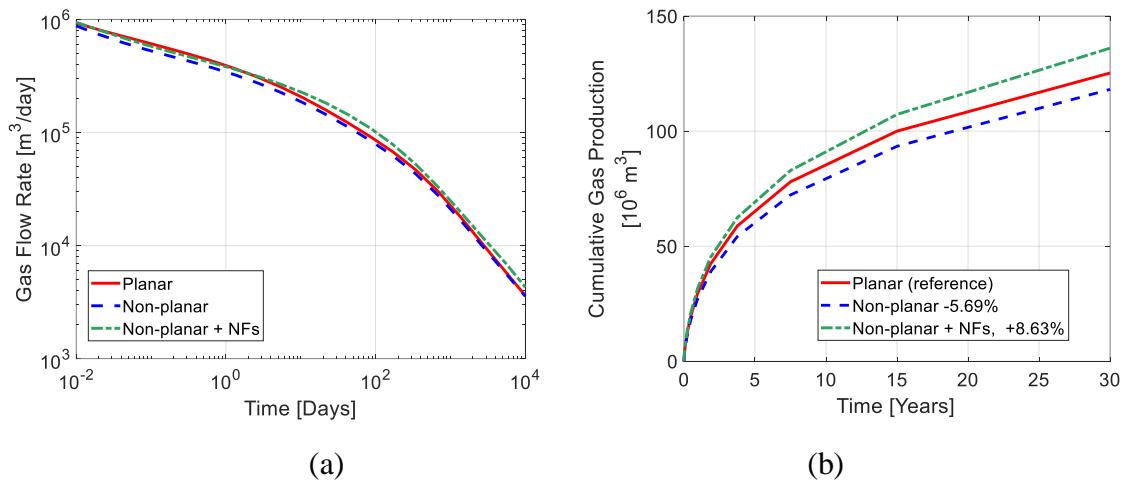


(a) Non-planar hydraulic fracture (Same total fracture length with Case 3)



1  
2 (b) Non-planar hydraulic fracture + natural fractures  
3  
4

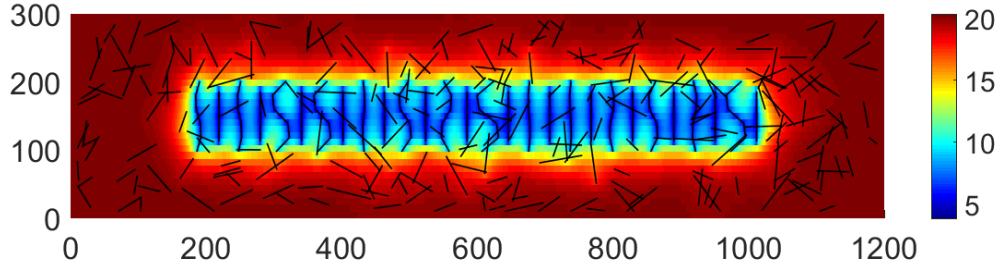
**Fig. 26 Pressure contour at the 3.75 years for Barnett shale reservoir with Non-planar fracture geometries and natural fractures (case 4)**



5  
6 (a)  
7 (b)  
8  
9

**Fig. 27 Comparison of gas flow rate (a) and cumulative production (b) between Planar,  
10 Non-planar and Non-planar & natural fractures cases**

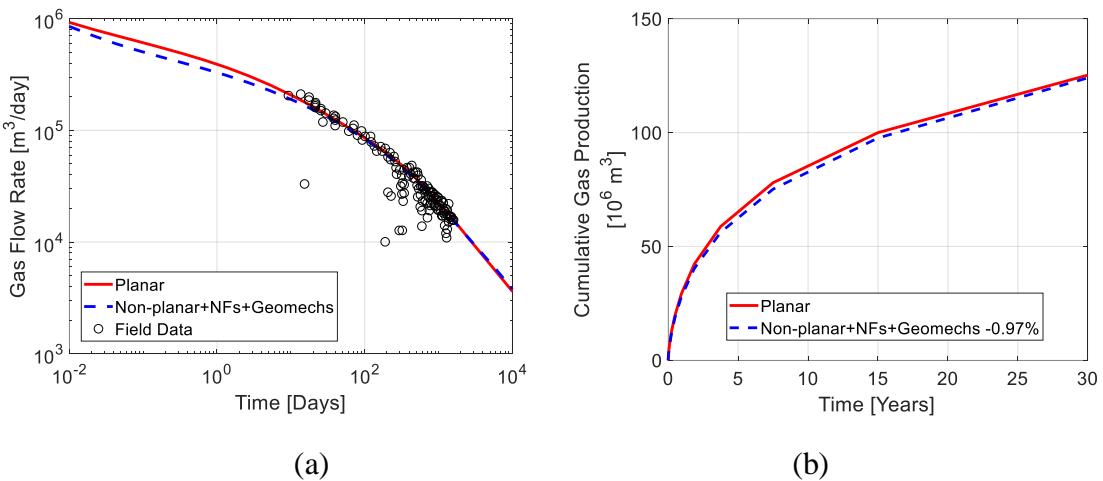
11 Firstly, the effect of complex fracture network on well performance is studied. **Fig 26** shows the  
12 pressure contour for the non-planar fractures with and without the natural fractures. Obviously, the  
13 case of natural fractures has larger and better stimulated reservoir volume (SRV). Thus, as shown in  
14 **Fig. 27**, the cumulative gas production of non-planar case with natural fracture has much higher  
15 value (14.56% improvements) than the planar case in the Case 3. While in the case of same total  
length, the non-planar fracture geometries will slightly degenerate the well performance (-5.69%  
reduction).



Non-planar hydraulic fracture + natural fractures + geomechanics effect

**Fig. 28 Pressure contour at 3.75 years for Barnett shale reservoir with planar hydraulic fractures case and realistic case**

The influence of geomechanics effect with fracture closure on well performance is further investigated by implementing Eqs. 15-17. **Fig. 28** shows the pressure contour at the 3.75 years for the planar case (Fig. 20a) and realistic case (Fig. 20b) with non-planar hydraulic fracture, natural fractures and geomechanics effect. As shown in **Fig. 29**, at the earlier production period, even realistic case has lower production than simple planar case due to geomechanics effect. But in the later production time, the contribution of natural fractures makes identical well performance between realistic case and simple planar case. Thus, the modeling of natural fractures and geomechanics effect is important for long-term production evaluation.



**Fig. 29 Comparison of gas flow rate (a) and cumulative production (b) between planar hydraulic fracture case and realistic case with non-planar, natural fractures and geomechanics effect**

## 6 Conclusion

In this work, A generic numerical model and an open-source framework OpenShale are developed for shale gas simulation with state-of-art flow and storage mechanisms. It is verified

1 against commercial and in-house reservoir simulators. The limitation of EDFM are also investigated  
2 quantity. Also, a field application of history matching and new model evaluation of geomechanics  
3 effect are successful performed. Several conclusions can be drawn as follows:

4 (1) A generic shale gas numerical model is developed which can be used to model any  
5 state-of-art storage and transport mechanisms, including gas adsorption, gas slippage &  
6 diffusion, non-Darcy flow as well as geomechanics effect by considering complex multi-scale  
7 fracture geometries.

8 (2) A general and open-source framework, OpenShale is developed and verified. With the help of  
9 the EDFM, Automatic Differentiation, and object-designed framework of OpenShale, one can  
10 easily use and extend OpenShale to simulate practical shale gas problem with arbitrary  
11 fracture geometries and new storage and transport mechanisms.

12 (3) EDFM can efficiently and accurately model irregular fracture geometry and complex fracture  
13 networks. However, it cannot accurately model low-permeability fracture (error of 12.22%)  
14 and hydraulic fractures without help of LGR where have strong transient behavior and sharp  
15 gradient (error of 2.84%). Thus, projected EDFM and adaptively grid refinement will be  
16 implemented and tested in our future work.

17 (4) Shale gas transport and storage mechanisms, such as gas desorption and gas slippage  
18 &diffusion flow gas, are the most significant impact on well performance, follow by natural  
19 fractures, geomechanics effect and fracture geometry.

20 (5) OpenShale is capable of serving as an efficient, flexible research tool to evaluate new models  
21 with arbitrary non-linearity and fracture complexity. It can serve as a bridge between  
22 mechanism study and field scale engineering application.

## 23

## 24 Nomenclature

25  $\rho_g$  = mass density of natural gas, kg/m<sup>3</sup>

26  $\phi$  = absolute rock porosity, dimensionless

27  $\Omega_m$  = matrix domain

28  $\Omega_f$  = fracture domain

29  $m_{ad}$  = storage mechanism term, kg/m<sup>3</sup>

30  $F_{app}$  = transport mechanism term, dimensionless

31  $k_0$  = absolute Darcy rock permeability, m<sup>2</sup>

32  $\mu_g$  = viscosity of natural gas, Pa·s

- 1         $p$  = pore pressure, Pa  
 2         $q_w$  = volumetric sink/source term, m<sup>3</sup>/day  
 3         $b_g$  = inverse formation volume factor, dimensionless  
 4         $M$  = molecular weight of natural gas, kg/mol  
 5         $Z$  = compressibility factor of natural gas, dimensionless  
 6         $R$  = ideal gas constant, 8.314 J/(mol·K)  
 7         $T$  = reservoir temperature, K  
 8         $T_{pr}$  = pseudo-temperature for natural gas, dimensionless  
 9         $T_c$  = critical-temperature for natural gas, K  
 10       $p_{pr}$  = pseudo-pressure for natural gas, dimensionless  
 11       $p_c$  = critical-pressure for natural gas, Pa  
 12       $a_{0,1,2}$  = constants for Peng-Robinson equation of state, dimensionless  
 13       $a, b$  = constants for Peng-Robinson equation of state, dimensionless  
 14       $A, B$  = constants for Peng-Robinson equation of state, dimensionless  
 15       $K, X, Y$  = constants for Lee-Conzalez-Eakin natural gas viscosity, dimensionless  
 16       $\rho_s$  = mass density of bulk matrix, kg/m<sup>3</sup>  
 17       $\rho_{gsc}$  = mass density of natural gas at the standard condition, kg/m<sup>3</sup>  
 18       $V_L$  = Langmuir volume, m<sup>3</sup>/kg  
 19       $P_L$  = Langmuir pressure, Pa  
 20       $V_m$  = BET volume, m<sup>3</sup>/kg  
 21       $P_s$  = BET pseudo-saturation pressure, Pa  
 22       $p_r$  = psdueo-pressure for BET isotherm, dimensionless  
 23       $C$  = constant for BET isotherm, dimensionless  
 24       $n$  = constant for BET isotherm, dimensionless  
 25       $\alpha$  = rarefaction coefficient for gas slippage flow, dimensionless  
 26       $K_n$  = Knudsen number, dimensionless  
 27       $\beta$  = Darcy-Forchheimer coefficient, dimensionless  
 28       $\alpha_B$  = Biot's coefficient, dimensionless  
 29       $P_c$  = reservoir confining overburden pressure, Pa  
 30       $P_I$  = reservoir effective stress when micro-fracture completely closed, Pa  
 31       $m$  = constant for the Gangi's model, Pa  
 32       $F_{cd}$  = fracture conductivity, md·ft  
 33       $p_0$  = initial reservoir pressure, m  
 34       $\sigma$  = effective fracture closure stress, Pa  
 35       $\sigma_{hf}$  = effective closure stress for hydraulic fracture, Pa  
 36       $\sigma_{nf}$  = effective closure stress for natural fracture, Pa  
 37       $\sigma_h$  = reservoir horizontal principle stress, Pa  
 38       $\sigma_{hmin}$  = minimum reservoir horizontal principle stress, Pa  
 39       $\sigma_{hmax}$  = maximum reservoir horizontal principle stress, Pa  
 40       $k_f$  = absolute Darcy permeability of fracture, m<sup>2</sup>  
 41       $w_f$  = fracture width, m  
 42       $V$  = bulk volume of a grid cell, m  
 43       $\delta$  = discrete domain delta function, dimensionless  
 44       $\Delta t$  = solution time-step, day

1       $\psi_{f-m}$  = mass coupling term for matrix, dimensionless  
 2       $\psi_{m-f}$  = mass coupling term for fracture, dimensionless  
 3       $p_{bh}$  = wellbore bottom hole pressure, Pa  
 4       $k_{11}$  = absolute Darcy rock permeability in x-direction, m<sup>2</sup>  
 5       $k_{22}$  = absolute Darcy rock permeability in y-direction, m<sup>2</sup>  
 6       $r_e$  = equivalent radius for wellbore model, m  
 7       $r_w$  = wellbore radius, m  
 8       $s$  = wellbore skin factor, dimensionless  
 9       $\Delta x$  = grid cell size in x-direction, m  
 10      $\Delta y$  = grid cell size in y-direction, m  
 11      $\Delta z$  = grid cell size in z-direction, m  
 12      $WI$  = wellbore index, dimensionless  
 13      $\mathbf{x}$  = Unknown vector, -  
 14      $\mathbf{J}$  = Jacobian matrix, -  
 15      $\mathbf{R}$  = Residual vector, -  
 16      $WI$  = wellbore index, dimensionless  
 17      $p_f$  = pore pressure at the fracture domain, Pa  
 18      $p_m$  = pore pressure at matrix domain, Pa  
 19      $T$  = transmissibility, dimensionless  
 20      $A$  = intersection area among fracture and matrix, m<sup>2</sup>  
 21      $d$  = average normal distance among fracture and matrix, m  
 22      $h_f$  = length of a fracture cell, m  
 23      $t$  = fracture transmissibility for fracture-fracture NNC, dimensionless  
 24

25 Subscripts:

26      $NF$  = natural fracture  
 27      $HF$  = hydraulic fracture  
 28      $m$  = matrix  
 29      $f$  = fracture  
 30      $g$  = gas  
 31      $w$  = well  
 32

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