Numerical Simulation of Shale Gas Flow in Three-Dimensional Fractured Porous Media

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Abstract

In this study, a Computational Fluid Dynamics (CFD) solver able to simulate shale gas flow as fluid flow in a porous medium on the macro level is presented. The shale gas flow is described by means of a tailored governing equation with both fluid properties and permeability expressed as a function of the effective pore pressure (stress effect) and with Knudsen effects included through an apparent permeability. This CFD solver, developed in the Open-Foam framework, allows for the simulation of three-dimensional fractured geometries without limitations on the shape of the domain. The solver was assessed and validated against literature data showing good agreement in terms of both recovery rate and pressure field profiles. The solver was then used to explore two different phenomena affecting shale gas dynamics: the diffusion behaviour and the influence of fracture geometry. It was shown that shale gas flow, on the macro level, is a diffusion-dominated phenomenon, and its behaviour can also be qualitatively represented by a diffusion equation. It was also shown that the early behaviour of shale gas flow is dictated by the fracture geometry, and that the reservoir dimensions have no effect on the flow at early times. Finally, a newly developed "dual-zone" solver, where the shale matrix and the fracture network are modelled as two distinct domains interacting through the common boundaries, is presented and discussed.

Keywords: Shale gas, Numerical simulation, CFD, OpenFoam, Coupled matrix and fracture zones

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1 1. Introduction

In recent years, there has been a renewed interest into alternative hy-2 drocarbon fuels (Youtsos et al. (2013)). Shale gas has become increasingly 3 important after the development of effective technologies for the extraction 4 of these trapped hydrocarbons (Mohaghegh (2013)). In addition to shale 5 gas, shale oil and oil shale constitute part of the current shale hydrocarbon 6 production. It is estimated that the world shale deposits contain around 3 7 trillion barrels worth of oil (Fan et al. (2010)). Because of this potential for 8 the future energy supply, there is a great interest from the energy industry 9 to improve the understanding of the flow of gas in tight and unconventional 10 reservoirs in order to be able to correctly predict production rates (Ma et al. 11 (2014)).12

Several attempts have been done in the past to model the gas flow in 13 shale and tight reservoirs, ranging from analytical and semi-analytical mod-14 els to numerical simulations. The very early analytical models involved very 15 simple geometries such as a single vertical fracture or a single horizontal 16 fracture (Gringarten et al. (1974)). These early models were followed by 17 semi-analytical models, such as the ones proposed by Patzek et al. (2013) 18 and by Blasingame and Poe (1993). Patzek et al. (2013) studied a very 19 simple configuration of the Barnett shale through a model derived from a 20 non-linear diffusion equation. Desorption was neglected and results were 21 compared with data extracted from real wells giving some insight into the 22 dominant parameters which affect the asymptotic behaviour of the reservoir 23 depletion. Although very fast, most of the analytical and semi-analytical 24 models suffer to capture the non-linearity in shale gas compressibility, viscos-25 ity, and compressibility factor due to the use of a pseudo-pressure approach, 26 rather than solving the real gas equation (Houze et al. (2010)). Furthermore, 27 these models also have difficulties in reproducing the typical characteristics 28 of shale gas reservoirs which involve desorption, multiphase flows and com-29 plex geometries (Houze et al. (2010)). Recently, some attempts to include 30 non-linearities of shale gas properties in analytical models have been per-31 formed (Ma et al. (2014); Wu et al. (2015)), however the applicability to 32 complex reservoirs needs further assessment and there is still need for an 33 approach able to give more detailed information about the shale flow in com-34 pletely three-dimensional domains. 35

In this scenario, numerical simulations offer the possibility to capture the non-linearities that in general analytical methods fail to adequately model

as well as the possibility of accurately reproducing complex reservoir shapes. 38 Furthermore, numerical simulations can be extensively used to perform a 39 sensitivity analysis on the main parameters that affect shale gas production. 40 The main limitations of numerical simulations are related to the compu-41 tational cost which however is mitigated by the increasing availability of 42 computational resources. Numerical simulations based on a finite element 43 approach were shown to be able to match historic production data of shale 44 gas (Miller et al. (2010); Jayakumar et al. (2011)). Cipolla et al. (2009) in-45 vestigated some of the parameters which may affect the gas flow, such as 46 the description of the flow from the matrix to the fracture network, stress 47 sensitive fracture conductivity, and desorption. A discrete approach to the 48 grid rather than a dual porosity model approach was utilized and it was 49 concluded that desorption might not be of importance in certain shale reser-50 voirs, but important in others. It was also concluded that the stress effect 51 on the fracture network is more evident during later stages of production 52 rather than at earlier stages and this could lead to optimistic production 53 forecasts (Cipolla et al. (2009)). Further understanding of the shale flow 54 was achieved by Freeman et al. (2013). The major parameters of shale flow 55 were identified as the ultra-tight permeability of shale, configuration of the 56 hydraulically fractured horizontal wells, multiple porosity and permeability 57 fields, and desorption (Freeman et al. (2013)). In addition, three regimes of 58 flow in typical fractured shale reservoirs were noticed: formation linear flow, 59 transitioning into compound formation linear flow, and eventually transform-60 ing into elliptical flow (Freeman et al. (2013)). It was also concluded that due 61 to the very low permeability in shale, the flow is controlled by the configura-62 tion of the fracture network, with and without desorption effects (Freeman 63 et al. (2013)). Furthermore, Moridis et al. (2010) explored the difference be-64 tween shale gas reservoirs and tight sand reservoirs using a multiphase solver 65 based on the Darcy equation. It was concluded that these types of reservoirs 66 differ from each other in the contribution of desorption. While desorption 67 can be neglected for tight sand reservoirs, significant deviations from field 68 data are observed if desorption is neglected for shale (Moridis and Freeman 69 (2014)).70

Earlier, Kwon et al. (2001) suggested that shale permeability of the Wilcox shale is a function of effective pressure. It was noticed that permeability decreased from 300×10^{-21} m² to 3×10^{-21} m² when the effective pore pressure increased from 3 MPa to 12 MPa. A cubic power pressure dependent equation of permeability was introduced to best fit the experimental

values of shale permeability (Kwon et al. (2001)). Later on, Freeman et al. 76 (2011) explored the compositional change of natural gas from shale reservoirs 77 with time. Many reasons were suggested for this phenomenon, but the most 78 important ones are the selective desorption from the surface of the matrix 79 and the non-Darcy flow which is the result of the nano-pores of shale. A 80 dependency between the natural gas composition and the Knudsen number 81 (which controls the non-Darcy flow) and eventually the permeability was 82 suggested. Freeman et al. (2011) placed a large importance on the Knudsen 83 number and used it to alter permeability into an apparent permeability as 84 suggested by Klinkenberg (1941) and Javadpour (2009). Apparent perme-85 ability allows retaining the form of the Darcy equation, while capturing the 86 Knudsen effect within the apparent permeability (Freeman et al. (2011)). 87 Further efforts in the understanding and modelling of shale gas flow include 88 a sensitivity analysis of the fracture geometry (Yu et al. (2014)), the use of 80 the finite elements method (Fan et al. (2015)), and a numerical solver that 90 includes slip flow, Knudsen diffusion, and desorption (Shabro et al. (2012)). 91 Although some aspects of shale gas flow have been already investigated. 92 there is still need of improving the knowledge of shale gas flow in geometries 93 close to the intricate configurations represented by the fracture network of 94 real reservoirs. In order to do that, a solver able to accurately model the 95 shale flow in every kind of geometry is required. In this work a new solver for 96 shale gas flow predictions is proposed and assessed with the main aim of: (i) 97 developing a numerical method able to solve a generic three-dimensional shale 98 reservoir, (ii) analyse the sensitivity of shale gas flow to the shape and the 90 physical properties of the reservoir. The newly developed tools also include a 100 dual domain approach where both the matrix and the fracture are included 101 in the domain and modelled as media with different properties interacting 102 through the common boundaries, offering hence greater accuracy in the flow 103 rate prediction as a function of fracture geometry. Both the mathematical 104

model and the approach used for shale gas simulation make the proposed
approach different from the existent commercial solver and models available
in literature.

108 2. Method

Shale reservoirs usually consist of a porous material (which in the following will be referred to as *matrix*) perforated by an intricate network of *fractures* used to collect the gas trapped in the pores. Despite the porous nature of the matrix, the shale gas flow has some peculiarities and cannot bedescribed as the typical flow in porous media.

The major factors affecting shale gas production modelling and even-114 tually forecast are identified as follows. The shale reservoir has a ultra-low 115 permeability and nano-pores, which could lead to a Knudsen diffusion contri-116 bution to the flow. This suggests the use of an apparent permeability which 117 includes matrix permeability as well as Knudsen diffusion effects (Javadpour 118 (2009)), while maintaining the use of a Darcy equation. The permeability de-119 pends on the effective pressure (stress effect), which is the difference between 120 confining pressure and pore pressure (Kwon et al. (2001)). Due to the ultra-121 low permeability, the fracture network has the largest influence on how the 122 flow proceeds. Finally no consensus has been reached on the role of adsorp-123 tion. Hill and Nelson (2000) suggest that 20% to 85% of total shale storage 124 is in the form of adsorption, however the majority may never be produced. 125 Others suggest that it could be neglected for certain reservoirs (Patzek et al. 126 (2013)). In this work the desorption of shale gas is not considered. This 127 choice is motivated by the fact that, according to the literature (e.g. Patzek 128 et al. (2013)) in the cases used for validation (Barnett shale) the desorption 129 can be neglected. However, it is important to point out that the approach 130 presented here is in principle not limited to cases without desorption since 131 this phenomenon can be included in the formulation through the Langmuir 132 isothermal theory (Shabro et al. (2012)). This will be attempted in future 133 works. 134

Starting from the typical equations describing the fluid dynamics, a math-135 ematical model for the shale gas flow can be derived (Chen et al. (2006); 136 Gruber (2014)). The following assumptions are considered in the following: 137 (a) single phase flow; (b) gas is assumed to be pure methane (single species); 138 (c) isothermal conditions; (d) negligible gravitational effects; (e) no sources 139 or sinks within the shale matrix; (f) porosity constant in time; (g) perme-140 ability is treated as a scalar (isotropic matrix); (h) permeability is a function 141 of effective pressure; (i) no desorption (the gas is only stored within the pore 142 spaces). In the following the mathematical model used in this work is first 143 presented followed by a description of the developed numerical solver and the 144 models adopted for shale properties. All the symbols are defined in Appendix 145 146 С.

147 2.1. Mathematical model

The typical representation of a continuum in Computational Fluid Dy-148 namics (CFD) problems, generally involves equations representing the con-149 servation of mass, species, momentum and energy. Since the flow considered 150 here is isothermal and single species (see assumptions (b) and (c)), trans-151 port equations for the conservation of energy and specific species are not 152 required (the conservation of methane is expressed through the conservation 153 of mass). In addition, capillary pressures and saturation equations are also 154 not required, because saturation is naturally set to one, with a single phase 155 single species flow. 156

Following Chen et al. (2006), the conservation of mass can be expressed as:

$$\frac{\partial \phi \rho}{\partial t} = -\nabla \cdot (\rho u) \tag{1}$$

where ϕ is the porosity, ρ is the density and the source terms on the right 159 hand side have been neglected because of assumption (e). The second equa-160 tion needed to completely describe the flow within the shale, is the momen-161 tum equation. However, since shale is a porous medium, the momentum 162 equation is replaced with the Darcy equation of velocity, which is an empir-163 ical equation derived originally for modelling water transport through sand 164 beds. Originally established by Henry Darcy in 1856, this law shows a linear 165 relationship between the fluid velocity and the pressure head gradient (Chen 166 et al. (2006)): 167

$$u = -\frac{1}{\mu}k(\nabla P - \rho g \nabla h) \tag{2}$$

where, P is the pressure, μ is the fluid viscosity, and k is the permeability. Applying assumption (d) to Eq. 2 yields:

$$u = -\frac{1}{\mu}k(\nabla P) \tag{3}$$

In order to close the system, an equation of state is also needed. While in the oil and gas industry cubic equations of state such as the Peng and Robinson (1975) and Soave (1972) equations of state are very common, in this work a real gas law exploiting the Standing and Katz (1942) empirical relationship for the compressibility factor z of natural gas is used (ERCB (1979); Mahmoud (2013)):

$$\rho = \frac{PW}{zRT} \tag{4}$$

where, W is the molecular weight, T is the temperature, and R is the methane gas constant. Since the fluid of interest is natural gas, which is a compressible gas, a compressibility C_q equation should be introduced:

$$C_g = \left(\frac{1}{\rho}\frac{\partial\rho}{\partial P}\right)\Big|_T \tag{5}$$

¹⁷⁹ Combining Eqs. 1, 3 and 4, a material balance for the gaseous species is ¹⁸⁰ obtained (Chen et al. (2006)):

$$\frac{\partial}{\partial t} \left(\frac{\phi PW}{zRT} \right) = -\nabla \cdot \left(\frac{PW}{zRT} \frac{1}{\mu} (-k) \nabla P \right) \tag{6}$$

¹⁸¹ Considering assumptions (c) and (f), Eq. 6 can be further simplified into:

$$\phi \frac{\partial}{\partial t} \left(\frac{P}{z} \right) = \nabla \cdot \left(\frac{Pk}{z\mu} \nabla P \right) \tag{7}$$

Generally (e.g. Patzek et al. (2013)), at this stage of derivation, the com-182 pressibility equation is incorporated in Eq. 7, and the pressures are replaced 183 with pseudo pressures (or P^2) to account for the error imposed by assuming 184 that the fluid properties (viscosity, compressibility, porosity, saturation) do 185 not depend on the pressure. However, in this paper, all the fluid properties 186 are taken to be pressure-dependent variables, and hence the need for pseudo 187 pressures is eliminated. As such, this paper takes a different direction, and 188 develops a tailored governing equation. Before further developing Eq. 7, Eq. 5 189 needs to be manipulated by introducing Eq. 4 and simplifying: 190

$$C_g = \frac{zRT}{PW} \left(\frac{W}{zRT} - \frac{PW}{z^2RT} \frac{dz}{dP} \right) = \frac{1}{P} - \frac{1}{z} \frac{dz}{dP}$$
(8)

Equation 8 can be expressed in the following form by multiplying by $\left(\frac{P\partial P}{z\partial t}\right)$:

$$C_g \frac{P\partial P}{z\partial t} = \frac{\partial P}{z\partial t} - \frac{P}{z^2} \frac{\partial z}{\partial t}$$
(9)

Finally, by replacing the right hand side of Eq. 9 with $\frac{\partial}{\partial t} \left(\frac{P}{z}\right)$, the final form of Eq. 5 is obtained.

$$\frac{\partial}{\partial t} \left(\frac{P}{z} \right) = \frac{\partial P}{\partial t} \frac{C_g P}{z} \tag{10}$$

Equation 10 is used to manipulate Eq. 7 into the final partial differential equation which describes shale gas flow. Using assumption (f), the right hand side of Eq. 10 can be equated to the right hand side of Eq. 7 multiplied by the porosity (ϕ), leading to:

$$\frac{\partial P}{\partial t} \frac{C_g P \phi}{z} = \nabla \cdot \left(\frac{Pk}{z\mu} \nabla P\right) \tag{11}$$

Rearrangement of Eq. 11 yields to the partial differential equation governing
 shale gas flow:

$$\frac{\partial P}{\partial t} = \frac{z}{C_g P \phi} \nabla \cdot \left(\frac{Pk}{z\mu} \nabla P\right) \tag{12}$$

200 2.2. Numerical Methods

Equation 12 has a similar structure to the diffusion equation (Gruber 201 (2014)) and therefore its implementation into a numerical solver is easier 202 than utilizing a pseudo-pressure equation. A solver for shale gas flow has 203 been implemented in the open source code OpenFOAM (Weller et al. (1998)) 204 where partial differential equations are solved by means of the finite volume 205 approach. The use of the OpenFOAM framework is very useful since it allows 206 for the solution of our model in every kind of geometry, without restrictions. 207 In addition, it allows the use of unstructured grids which facilitate the dis-208 cretization of complex geometries, typically found in shale gas applications. 209 In order to directly exploit the discretization of the differential operators 210 already available in OpenFOAM, Eq. 12 was rearranged in the following 211 equivalent form which allows an easier implementation: 212

$$\frac{\partial P}{\partial t} = \nabla \cdot \left(\frac{k}{\phi \mu C_g} \nabla P\right) - \nabla \left(\frac{k}{\phi \mu C_g}\right) \cdot \nabla P + \frac{z}{C_g P \phi} \nabla \left(\frac{Pk}{\mu z}\right) \cdot \nabla P \quad (13)$$

Once Eq. 13 is solved and the pressure is known, the Darcy velocity can be calculated through Eq. 2 and hence the flow rate can be found. It is important to point out that the reservoir and fluid properties appearing in Eq. 13 can in general be a function of both space and pressure. Permeability, compressibility, compressibility factor, and viscosity, are all treated as spatial variables rather than constants. In addition, these variables will be treated as pressure dependent, as discussed in Section 2.4.

In all the computations performed in this work, the time derivative was discretized using a backward Euler implicit scheme whereas central differencing second order schemes were used for spatial discretization. If not differently specified, all the computational grids used in this paper are hexahedral meshes (generated using the OpenFOAM meshing tool), but, exploiting
the unstructured formulation of the OpenFOAM framework, other meshing
strategies can also be used.

Equation 13 can be applied either (i) to the matrix only (single-zone 227 solver) or (ii) to both the matrix and the fracture (dual-zone solver) and 228 both these versions of the solver were implemented. The first case is the 229 simplest scenario where only the matrix needs to be discretized. Boundary 230 conditions are applied to (1) the reservoir confinement, where generally a 231 zero-gradient condition is assumed for the pressure to represent a wall with no 232 flux, but also different types of conditions such as cyclic or constant pressure 233 are possible, and (2) at the interface between the matrix and the fracture, 234 where a constant pressure is usually imposed. In the case of dual-zone solver 235 both the matrix and the fracture should be included in the computational 236 domain and different shale properties should be assigned to these two regions 237 (for example matrix and fracture have different porosity). In the approach 238 followed in this work, the matrix and the fracture were modelled as two 239 different domains interacting through specific boundary conditions at the 240 common interface. A detailed description of the dual-zone solver is given in 241 Section 2.3. 242

243 2.3. Dual Zone Solver

Petroleum reservoirs usually consists of a low permeability/low porosity 244 matrix and a network of relatively high permeability/high porosity fractures. 245 Historically, the fracture network was natural and, due to the difference in 246 the properties of the matrix and the fracture, this led to the development of 247 dual porosity and dual porosity/dual permeability models in order to better 248 represent the complex geometry of fractures inside a rock matrix (Chen et al. 240 (2006)). While such models were developed long time ago in order to better 250 represent petroleum reservoirs with natural fractures, there seems to be a 251 similar need for shale gas reservoirs, especially with the added complexity of 252 hydraulic fractures. 253

It would be useful to extend the solver to allow the simulation of the gas flow in both the shale matrix and the fracture network. In order to do that, a *dual-zone* solver has been implemented where the matrix and the fracture network are treated as two distinct domains, each with its own governing equation and parameters (including permeability and porosity), that only interact at their common boundary. This approach is different from the dual porosity model, where the matrix is resembled by blocks and the fracture is resembled by spaces in between the matrix blocks (Chen et al. (2006)), and in principle does not need any transformation or simplification. This offers a great advantage into simulating realistic fracture networks. The dual solver was implemented starting from the dual-zone heat transfer solver developed by Craven and Campbell (2011) for conjugate heat transfer problems.

266 2.3.1. Governing Equations

While the flow within a fracture has been studied and treated as a Navier-267 Stokes flow in many studies (Brush and Thomson (2003); Zimmerman and 268 Bodvarsson (1996)), the dual porosity model treats the flow within the frac-269 ture as a flow inside a porous medium (Chen et al. (2006)). The fracture is 270 usually characterized by the presence of rock residuals or proppants which 271 in general should be taken into account for an accurate prediction of the 272 flow (Chen et al. (2006)). If Navier-Stokes equations are used, the effect of 273 rock residuals can be included in the simulation only thorough the geometry 274 resulting in a very complex shape of the fracture domain. However, if the 275 flow inside the fracture is treated as a porous medium, the Darcy equation 276 can be used and the effect of rock inside the flow can be taken into account 277 through porosity and permeability values. As a result, in this work the two 278 domains will be treated as porous media with the same governing equation 279 (see Eq. 13). The interaction between these two domains will be controlled 280 through the coupling done at the common boundary. The specific boundary 281 conditions applied to the matrix and the fracture at the common interface 282 are detailed in Sections 2.3.2 and 2.3.3. 283

284 2.3.2. Matrix Boundary Condition

The boundary condition applied to the matrix at the interface I with the fracture is expressed in terms of pressure. The pressure seen by the matrix should be equal to the pressure on the fracture side. This is a Dirichlet boundary condition and reads as:

$$P_m|_I = P_f|_I \tag{14}$$

289 2.3.3. Fracture Boundary Condition

Inspired by the dual porosity model, which states that the flow rate of the gas leaving the matrix enters the fracture network, the boundary condition

for the fracture, at the fracture-matrix interface, is a Neumann boundary condition. The introduction of the mass flow rate leaving the matrix into the fracture as a boundary condition is done through the pressure gradient. By imposing that the mass flow rate leaving the matrix is equal to the flow entering the fracture and after introducing the Darcy expression (Eq. 2) for the velocity and removing the area which is a common factor, the following expression for the boundary condition at the common interface I is obtained:

$$\dot{m}_f|_I = \dot{m}_m|_I \to \rho_f A u_{f,n} = \rho_m A u_{m,n}$$
$$\to \rho_f \frac{k_f}{\mu_f} \nabla P_{f,n}|_I = \rho_m \frac{k_m}{\mu_m} \nabla P_{m,n}|_I \quad (15)$$

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$$\nabla P_{f,n}|_{I} = \frac{\rho_m}{\rho_f} \frac{k_m}{k_f} \frac{\mu_m}{\mu_f} \nabla P_{m,n}|_{I}$$
(16)

Hence the coupling is done by imposing on the fracture side the component of the pressure gradient normal to the interface according to Eq. 16. If this coupling algorithm is working properly within the solver, considering also that at the interface the matrix and the fracture have the same pressure (see Eq. 14) and therefore the same density, the normal component of the Darcy velocity at the common boundary should be be equal for each zone. This will be used later on for validation.

298 2.4. Natural Gas and Shale Properties

In order to properly describe the evolution of shale gas, physical proper-299 ties appearing in Eq. 13 need to be accurately modelled. In the following, the 300 main modelling assumptions for the physical properties of shale gas (methane 301 is considered here) are summarized together with some considerations regard-302 ing the porosity and permeability of the matrix. It is important to point out 303 that the code is not limited to the use of the following relations. In prin-304 ciple, every kind of relation for the physical properties can be implemented 305 and used making the approach very flexible and ready to incorporate a more 306 comprehensive description of the properties or to be extended to different 307 fuels and applications. 308

309 2.4.1. Compressibility factor

Methane has a critical temperature of 190 K and a critical pressure of 4600 kPa (Friend et al. (1989)). The pressure and temperature of the natural gas found within shale formations exceeds the critical values. Hence,

methane will not behave as an ideal gas within shale. Originally, Standing 313 and Katz (ERCB (1979)) developed plots of the compressibility factor for 314 sweet natural gas versus reduced pressure and temperature. These charts 315 were curve-fit by Dranchuk, Purvis, and Robinson, using the BWR equa-316 tion of state (ERCB (1979)). However, Mahmoud (2013) showed that the 317 original equations are not accurate at high pressures, and suggested another 318 set of equations which better matches compressibility factor values at high 319 pressure. 320

$$z = aP_r^2 + bP_r + c$$

$$a = 0.702e^{-2.5T_r}$$

$$b = -5.524e^{-2.5T_r}$$

$$c = 0.044T_r^2 - 0.164T_r + 1.15$$

(17)

³²¹ where the reduced pressure and the reduced temperature are given by:

$$P_r = \frac{P}{P_{cr}}, \quad T_r = \frac{T}{T_{cr}} \tag{18}$$

Furthermore, Jarrahian et al. proposed a cubic equation of state which allows the calculation of the compressibility factor of natural gas with higher accuracy (Jarrahian and Heidaryan (2014)), and can be seen in Appendix B. In this code, due to the flexibility of the OpenFOAM framework, any adequate equation of state can be implemented, depending on the composition of the gas and the properties of the reservoir.

As a result, compressibility factor was implemented into the code as a pressure dependent property using both, Eq. 17 (Mahmoud (2013)) and Eq. B.1 (Jarrahian and Heidaryan (2014)) (Eq. B.1 is the virial form of the cubic equation of state presented in Jarrahian and Heidaryan (2014)). The results shown in Section 3 were produced using Eq. 17, while the results produced using Eq B.1 are included in Appendix A.

334 2.4.2. Compressibility

Similar to the compressibility factor, compressibility has an empirical equation which was developed by Dranchuk, Purvis, and Robinson (ERCB (1979)). However, since compressibility can be calculated from the equation of compressibility factor (Eq. 17), we will use the relation presented by Mahmoud (2013), which provides better accuracy at high pressures. The compressibility is described by the following set of equations (Mahmoud (2013)):

$$C_{g} = \frac{C_{r}}{P_{r}}$$

$$C_{r} = \frac{1}{P_{r}} - \frac{1}{z} \left(\frac{\partial z}{\partial \rho_{r}}\right)_{T_{r}}$$

$$C_{r} = \frac{1}{P_{r}} - \frac{1}{z} [P_{r}(1.404e^{-2.5T_{r}}) - (5.524e^{-2.5T_{r}})]$$
(19)

where the reduced pressure P_r and reduced temperature T_r were defined in 335 Eq. 18. In Fig. 1, the compressibility and compressibility factor predicted 336 using Eqs. 17, B.1 and 19 are compared with the equations suggested by 337 Dranchuk, Purvis, and Robinson (ERCB (1979)). The three methods give 338 very similar values for a reduced pressure less than 1.0 whereas for higher 330 pressures (pressure larger than the critical value) the effect of the corrections 340 suggested by Jarrahian and Heidaryan (2014) and by Mahmoud (2013) is 341 clearly visible. 342

343 2.4.3. Viscosity

The viscosity of natural gas, and in this case pure methane, varies by a factor of four between pore pressure and fracture pressure (Ling (2010)). Hence, for the sake of mathematical rigour as well as exploiting the advantage of numerical simulation, viscosity will also be pressure dependent. The Lee-Gonzalez-Eaken correlation (Gonzalez et al. (1970)) was developed by measuring the viscosity of eight natural gases over a range of temperatures and pressures. This correlation can be seen in Eq. 20 (Ling (2010)).



Figure 1: Compressibility factor and compressibility versus reduced pressure, produced using the equations from Refs. ERCB (1979), Jarrahian and Heidaryan (2014), and Mahmoud (2013).

$$\mu = 10^{-4} K \exp(X \rho^{Y})$$

$$K = \frac{(9.379 + 0.01607W)T^{1.5}}{209.2 + 19.26W + T}$$

$$X = 3.448 + \left[\frac{986.4}{T}\right] + 0.01009W$$

$$Y = 2.447 - 0.2224X$$

$$\rho = \frac{PW}{zRT} = 0.00149406\frac{PW}{zT}$$
(20)

where μ is in cp (centipoise), P in psia, ρ in g/cm³, and T in °R.

In addition, Jarrahian et al. (2015) suggested a different viscosity cor-352 relation, based on their own cubic equation of state, which provides better 353 accuracy at higher pressures and temperatures for sour and sweet natural 354 gases. This correlation can be seen in Eq. B.2 (Jarrahian et al. (2015)), and 355 can be found in Appendix B. The values of viscosity predicted by Eq. 20 356 and Eq. B.2 are shown in Fig. 2. The results shown in Section 3 were pro-357 duced using Eq. 20, while the results produced using Eq B.2 are included 358 in Appendix A. 359



Figure 2: Viscosity versus reduced pressure using Eq. 20 and Eq. B.2

360 2.4.4. Permeability

In general, reservoirs with permeability below 10^{-15} m² (1.013 mD) are 361 considered tight (Wang et al. (2014)). This dictates that shale, which is clas-362 sified as a tight reservoir, will have a permeability lower than 10^{-15} m² (1.013) 363 mD). So Soeder (1988) reported a shale permeability of 2×10^{-17} m² (20.26 364 μ D). Bruner et al. (2011) reported values within the range of 2 × 10⁻¹⁷ m² 365 $(20.26 \ \mu D)$ to $1 \times 10^{-16} \ m^2(100.13 \ \mu D)$. In 2006, the US geological sur-366 vey published a report which compiled shale sample results from several 367 shale formations. This report states that shales with liquid petroleum in 368 their pores had very low permeabilities in the range of tens of nano-darcies 369 $(1 \times 10^{-20} \text{ m}^2)$ (Milici and Swezev (2006)). With many shale reservoirs 370 containing oil and gas, permeabilities in the range of nano-darcies remain 371 realistic. Keeping in mind that hydraulic fractures are created to increase 372 permeability and that naturally occurring fractures passively increase per-373 meability, one cannot standardize a constant permeability for shale. Even 374 further, some works suggest that permeability depends on pressure. For ex-375 ample, the permeability of illite-rich shale of the Wilcox formation has been 376 found to decrease from $3 \times 10^{-19} \text{ m}^2$ (304 nD) to $3 \times 10^{-21} \text{ m}^2$ (3.04 nD) when 377 the effective pressure increases from 3 MPa to 12 MPa (Kwon et al. (2001)). 378 As a result, this paper utilizes a permeability equation which depends on 379 effective pressure (Kwon et al. (2001)): 380

$$k = 10^{-17} \left[1 - \left(\frac{P_e}{19.3 \times 10^6} \right)^{0.159} \right]^3 \tag{21}$$

The effective pressure, P_e , is the difference between confining pressure, the pressure due to the weight of the rock on top of the reservoir, and the pore pressure. Confining pressure P_c is estimated at 38 MPa throughout the paper.

In addition, as noted in Section 1, it was suggested that the Darcy equa-384 tion for velocity is not sufficient to represent shale gas flow, which is a slip-flow 385 or a transition flow. However, Javadpour (2009) showed that we can indeed 386 maintain the Darcy form, but we need to use a specific form of permeability, 387 called apparent permeability, which takes into account both the effect of the 388 physical geometry of the rock (Darcy permeability) and the flow (slip and 380 Knudsen effects). Apparent permeability is also used in this paper according 390 to the following expression (Javadpour (2009)): 391

$$k_a = \frac{2r\mu W}{3 \times 10^3 RT \rho_{avg}^2} \left(\frac{8RT}{\pi W}\right)^{0.5} + \left(\frac{r^2}{8\rho_{avg}}\right) \left[1 + \left(\frac{8\pi RT}{W}\right)^{0.5} \frac{\mu}{p_{avg}r} \left(\frac{2}{\alpha} - 1\right)\right]$$
(22)

In Eq. 22, α is called the tangential momentum accommodation coefficient (the fraction of the gas molecules reflected diffusely), and ranges between 0 and 1.

The values of permeability given by Eqs. 21 and 22 as a function of pres-395 sure are shown in Fig. 3 (pore radius was assumed to be 2 nm, and α was 396 assumed to be 0.5). In Fig. 3(a), permeability increases as pressure increases. 397 Physically, this can be attributed to the aperture of the pores. As the pore 398 pressure increases, it resists against the confining pressure and keeps the 399 physical pore volume large, which enhances the flow and subsequently in-400 creases permeability (elastic deformation is minimal). On the other hand, as 401 the pore pressure decreases, the confining pressure starts to crush the pores, 402 decreasing their volume, and subsequently reduce permeability (elastic de-403 formation is significant) (Kwon et al. (2001)). In addition, when natural or 404 hydraulic fractures exist, the same effect can be noticed, which leads to the 405 use of proppant to maintain an adequate fracture aperture and to enhance 406 recovery. Nevertheless, the use of proppants does not infinitely improve re-407 covery, as the fractures and the proppant will eventually be crushed, and 408 this gives shale gas its characteristic sharp production drop which is usu-400 ally mitigated by drilling many wells. On the contrary, Fig. 3(b) shows that 410 the apparent permeability decreases as pressure increases. Permeability has 411 a value slightly smaller than $1 \times 10^{-19} \text{ m}^2$ (101 nD) for pressure equal to 412 35 MPa (this is the initial reservoir pressure throughout this paper), which 413 is the Darcy permeability. As discussed in (Javadpour (2009)), for pressures 414



Figure 3: Permeability versus pressure using Eqs. 21 and 22, from Refs. Kwon et al. (2001); Javadpour (2009).

larger than 10 MPa, the Darcy and the apparent permeability have a ratio 415 of 1.0. As pressure decreases, the ratio of apparent to Darcy permeability 416 increases significantly because the mean free path increases, and the flow 417 shifts into slip and Knudsen regimes. The apparent to Darcy permeability 418 ratio at the pressure of 5 MPa is around 5, as can be deduced from Fig. 3(b) 419 by comparing the permeability values at 35 MPa and 5 MPa. This observa-420 tion is consistent with results presented by Javadpour (2009). Finally, the 421 permeability resulting from the combined effects of pressure dependence and 422 apparent permeability is shown in Fig. 3(c). In order to combine both Eq. 21 423 and Eq. 22, the constant 10^{-17} in Eq. 21 was replaced by the permeability 424 calculated from Eq. 22. The term 10^{-17} can be seen as a base permeability 425 being adjusted by the pressure (stress effect). The permeability is equal to 426

the base value for $P_e = 0$ and decreases as the effective pressure increases. This effect is also replicated in Fig. 3(c), where the use of Eq. 22 for the base value results in lower values of the permeability. This should be considered an attempt to include both the stress and Knudsen effects in the same formulation.

432 2.4.5. Porosity

Although porosity is not a homogeneous and constant property, it is sim-433 pler to assume it as a constant, especially when the shale is assumed to be 434 isotropic (assumptions (f) and (g)). It was estimated that the average poros-435 ity of the Barnett and Marcellus shales is 6% (Bruner et al. (2011)). Other 436 sources suggest a range of porosity between 8.2% and 11.4% for the Marcel-437 lus shale (Taylor (2013)). As such, a value of 9% porosity will be used in 438 this study. Note, however, that our governing equation (Eq. 13) allows for ϕ 439 variations in space, if needed. 440

441 3. Results and Discussion

First, an assessment and validation of the model proposed here will be 442 presented followed by the analysis of the diffusion behaviour and the influence 443 of the fracture geometry. An example of simulation of a very complex frac-444 ture geometry is also included. Both the validation and the analysis of the 445 behaviour of shale gas flow were performed using the single-zone solver, where 44F only the matrix was included in the computational domain. The generic case 447 solved here includes a horizontal well, with two vertical orthogonal penny-448 shaped fractures, as shown in Fig. 4. Finally, an application of the dual-zone 440 solver, showing the potentiality of this approach, is presented and discussed. 450

451 3.1. Validation

The model is validated against two sets of literature results. The first one is the work of Patzek et al. (2013), where a two-regime flow is described. The second one is the work of Freeman et al. (2013), where the shale gas flow exhibits three types of flow: formation linear flow, compound linear flow, and elliptical flow.

457 3.1.1. Two-Regime Flow

In the work of Patzek et al. (2013) thousands of well data, from the Barnett, were analysed and compared with a one-dimensional model for shale



Figure 4: Generic fracture geometry.

gas production. It was shown that the fractional cumulative gas production (Recovery Factor, RF) before fracture interference is proportional to a factor κ multiplied by the square root of a normalized dimensionless (scaled) time \tilde{t} :

$$RF(\tilde{t}) \approx \kappa \sqrt{\tilde{t}}$$

$$\tilde{t} \equiv t/\tau \quad , \quad \tau = d^2/\alpha_i$$

$$\alpha_i = \frac{k}{\phi S_g \mu_g C_g} \bigg|_{Initial \ reservoir \ P, \ T} \quad , \quad RF(\tilde{t}) = m/M$$
(23)

where τ is the time elapsed before the occurrence of fracture interference, 458 which depends on the initial conditions of the reservoir as well as the dis-459 tance between two adjacent fractures but not on the reservoir dimensions. 460 It was also shown that the recovery rate (or mass flow rate) exhibits a two-461 regime flow. In the first regime, the recovery rate declines at a rate inversely 462 proportional to the square root of the dimensionless (scaled) time. The sec-463 ond regime is an exponential decline which occurs after fracture interference. 464 The one-dimensional model proposed by Patzek et al. (2013) is based on 465 the same governing equations described in this study, but with a different 466 treatment of the pressure dependence of the shale properties for which a 467 pseudo-pressure notation was introduced. On the other hand, the formula-468 tion proposed in this work solves for the flow in three dimensions, retain-469 ing the governing equation in absolute pressure form (without resorting to 470

⁴⁷¹ pseudo pressures because all the fluid properties are implemented as functions



Figure 5: Schematic of the two cases investigated for the assessment of the two-regime flow.

of pressure). Since in the model derived in this work an isotropic matrix is
assumed, a behaviour similar to the one found by Patzek et al. (2013) is also
expected from our computations. Therefore, the capability of the present
approach to capture the two-regime flow will be evaluated in the following
as a first step of validation.

Two different cases were solved here as schematically shown in Fig. 5. 477 Both cases use the generic fracture geometry shown in Fig. 4 which is equiv-478 alent to the uniformly spaced hydrofracture stages in a horizontal well con-479 sidered in Patzek et al. (2013), and differ for the spacing between the fracture 480 elements and the dimension of the reservoir. The relevant properties of each 481 case are shown in Table 1. A uniform pressure equal to 5.0 MPa was imposed 482 at the fracture boundary whereas the zero-gradient condition (no outflow) 483 was applied at the reservoir walls. An initial pore pressure of 35.0 MPa was 484 applied in both cases. 485

While Patzek et al. (2013) assumed a constant permeability, deduced from Eq. 23 through a direct comparison with experimental measurements (for the investigated wells, a value in the range of 5×10^{-19} m²(506 nD) to 5×10^{-20} m² (50.6 nD)was found), here different permeability models (PM) were considered and applied to each case, therefore assessing the effect of permeability on the shale flow prediction. Table 2 summarizes the different permeability models used here. First, a constant permeability of 1×10^{-19} m² (101 nD)

Case	Case 1	Case 2
Total Length	5 m	5 m
Total Width	5 m	1.5 m
Total Height	5 m	5 m
Fracture Half Length	0.9 m	0.9 m
Fracture Spacing	1.0 m	0.5 m
Fracture Thickness	$3 \mathrm{mm}$	$3 \mathrm{mm}$
Porosity	9~%	9 %
α	0.5	0.5
Pore Radius	2 nm	2 nm
Temperature	330 K	330 K
Critical Pressure	4.6 MPa	4.6 MPa
Critical Temperature	190 K	190 K
Molar Mass (M_w)	16.04 kg/kmol	16.04 kg/kmol
Number of Elements	1.6 million elements	0.9 million elements
Time Step	60 seconds	60 seconds
Initial Pore Pressure	$35 \mathrm{MPa}$	$35 \mathrm{MPa}$
Outlet (Fracture) BC	Dirichlet (5 MPa or 25 MPa)	Dirichlet (5 MPa or 25 MPa)
Reservoir BC	Neumann (Zero-Gradient)	Neumann (Zero-Gradient)
Characteristic Time τ	8.44 hours or 844 hours	2.11 hours or 211 hours

Table 1: Properties of the two generic cases solved.

was assumed (PM1); second, the dependence on the effective pressure (stress effects, see Eq. 21 Kwon et al. (2001)) was accounted for (PM2); third, the apparent permeability (Knudsen effects, see Eq. 22 (Javadpour (2009))) was considered (PM3); finally, by combining Eq. 21 and Eq. 22, both the stress and Knudsen effects were included (PM4). An average pore radius r = 2 nm and tangential momentum accommodation coefficient $\alpha = 0.5$ were assumed, when using apparent permeability.

It is important to note that in reality, actual permeability values are larger 500 than the values experimentally tested in labs, due to the effect of hydraulic 501 fracturing on permeability values in the vicinity of the fracture/matrix in-502 terface (Patzek et al. (2013)). Equation 21 from Kwon et al. (2001), is a 503 lab-based relationship and because of that will provide permeability values 504 lower than actual wells. Therefore, it is expected that when this expression 505 is used, a lower recovery rate will be produced. This relation was tested for 506 an effective pressure range of 3 MPa to 12 MPa (Kwon et al. (2001)), and as 507 such, the boundary condition at the fracture surface was increased to 25 MPa 508 for PM2 and PM4, to maintain the effective pressure within the tested range. 509 Figure 6 shows a 3D cut of the computational mesh used for Case 1. 510

Table 2: Summary of the four permeability models (PM) used in this work.

Permeability Model (PM)	Main Feature
Permeability Model 1 (PM1)	Constant Permeability $(1 \times 10^{-19} \text{ m}^2)$ (101 nD)
Permeability Model 2 (PM2)	Stress Effect (Effective Pressure Permeability, Eq. 21 Kwon et al. (2001))
Permeability Model 3 (PM3)	Knudsen Effect(Apparent Permeability, Eq. 22 Javadpour (2009))
Permeability Model 4 (PM4)	Stress Effect and Knudsen Effect (Eq. 21 and Eq. 22)



Figure 6: Computational mesh used for Case 1.

Refinements around the fracture were adopted in order to properly solve 511 the pressure gradients, usually very steep in this region. A similar grid 512 was also used for Case 2 and for all the other cases investigated in this 513 work, except the complex fracture geometry presented in Section 3.4 for 514 which a tetrahedral mesh was used. An example of time evolution of the 515 pressure and permeability (PM3) inside the matrix is shown in Fig. 7 where 516 snapshots of the solution at different times are reported. As time advances, 517 the pressure around the fracture drops and hence the permeability increases, 518 which matches the trend in Fig. 3-b (Since PM3 is utilized in this case). 519 Although in Section 3, the solution is analysed mainly in terms of global 520 quantities (such as recovery rate and recovery factor), the outcome of the 521 solver is the three-dimensional pressure field which allows us to monitor the 522 evolution of the shale quantities in any region of the domain. 523

Since the fracture spacing in Case 1 is double the one in Case 2 (1.0 m and 0.5 m, respectively), the characteristic time τ for Case 1 is four times the characteristic time for Case 2 because the fracture spacing in Eq. 23 is squared. With the initial pore pressure of 35 MPa and initial reservoir temperature of 330 K (Table 1), the two cases investigated here have a characteristic interference time τ of 8.44 and 2.11 hours respectively, for PM1-PM3.



Figure 7: Pressure and permeability plots at several times, for Case 1 using PM3

⁵³⁰ However, for PM4, when permeability at the initial conditions is 1×10^{-21} m² ⁵³¹ (1.01 nD), see Fig. 3(c), interference time τ increases to 844 and 211 hours ⁵³² respectively.

Figures 8 and 10 show the recovery factor and the recovery rate versus the scaled time, obtained for Case 1 using the different permeability models.



Figure 8: Recovery factor versus scaled time for Case 1 predicted using the four permeability models (PM), with curve matching.

Similarly, results for Case 2 are reported in Figs. 9 and 11. All the results 535 show an agreement with the two-regime flow previously described and for 536 both Case 1 and Case 2, the use of apparent permeability (PM3) allows for 537 a better match of the profile inversely proportional to the square root of the 538 scaled time observed by Patzek et al. (2013) before fracture interference. Ap-539 parent permeability is the key feature that distinguishes the shale gas flow 540 from other porous material, and in general should be included in the formu-541 lation. It is also interesting to note that the recovery rate and recovery factor 542 are very sensitive to the value of the permeability and different predictions 543 are obtained with the various models. Therefore, great attention should be 544 devoted to the selection of the right model for permeability. 545

It is also interesting to look at the value of the constant κ appearing in



Figure 9: Recovery factor versus scaled time for Case 2 predicted using the four permeability models (PM), with curve matching.

the expression of the recovery factor vs. scaled time during the early stages 547 of the reservoir depletion (Eq. 23). This constant depends on the fracture 548 geometry, the permeability of the shale, the gas properties, as well as the 549 reservoir size. For the Barnet shale wells, a value around 0.625 was found 550 by Patzek et al. (2013) whereas for the geometries investigated in this work 551 a value in the range 0.001-0.015 seems to give a good scaling. Assuming 552 that in real application the fracture network is created through hydraulic 553 fracturing, for optimal (fastest) recovery, $\kappa = 0.625$ can be regarded as a 554 practical (rather than theoretical) upper limit. The fracture networks used 555 in this paper are far from being optimized for recovery. Hence, κ is far lower 556 than the value suggested by Patzek et al. (2013). However, when comparing 557 the two cases (see Fig. 8 and Fig. 9), it should be noted that Case 2 depletes 558



Figure 10: Recovery rate versus scaled time for Case 1 predicted using the four permeability models (PM), with curve matching.

⁵⁵⁹ much faster than Case 1. This can be attributed to the reservoir size and to ⁵⁶⁰ the characteristic interference time τ . For the same fracture network, a larger ⁵⁶¹ reservoir reduces the constant κ , because of the larger amount of natural gas ⁵⁶² in the reservoir, which naturally requires a longer time to extract. In addition, ⁵⁶³ a larger characteristic interference time τ reduces the constant κ , because it ⁵⁶⁴ takes a longer time for fracture interference to occur.

The results shown in this section demonstrate that the three-dimensional shale gas flow still preserves the two-regime flow characteristics described by Patzek et al. (2013), regardless of the model used to include the permeability. However, the recovery rate is in general very sensitive to the permeability, and therefore great care should be used for the selection of the more consistent permeability model, being both stress and Knudsen effects



Figure 11: Recovery rate versus scaled time for Case 2 predicted using the four permeability models (PM), with curve matching.

⁵⁷¹ in general non-negligible.

572 3.1.2. Three-Regime Pressure Contours

In the work of Freeman et al. (2013), the pressure field inside the matrix 573 was directly analysed and on the basis of the different shapes of the pres-574 sure iso-lines. Three flow regimes were distinguished: formation linear flow, 575 compound formation linear flow, and elliptical flow. In order to qualitatively 576 validate the solver presented in this study, the pressure contours obtained in 577 the previous simulations are compared to those presented by Freeman et al. 578 (2013). Although the dimensions of the fracture and the well network used 579 here are different compared to the geometry used in (Freeman et al. (2013)), 580 the trends of the pressure profiles can still be compared. Figure 12 shows 581



Figure 12: Left: formation linear flow, Center: compound linear flow, Right: elliptical flow Freeman et al. (2013). (Reused with persmission from Elsevier. License Number: 3902540332270)

the three flow regimes around the fracture from the work by Freeman et al. (2013). The linear flow seen in Fig. 12 is characterized by parallel pressure iso-lines. As the flow proceeds into compound linear and elliptical flow, the iso-lines spread around the fracture and are not parallel anymore but transform into elliptical profiles.

Fig. 13 shows the pressure profiles from the solution of Case 2 (using a variable permeability function). Qualitatively, the same transition into the three regimes of Fig. 12 was found. While the geometric dimensions are different between the two studies, the comparison demonstrate the capability of the present approach to capture the required physics, showing agreement with literature pressure regimes around the fracture.

Furthermore, Freeman et al. (2013) suggest that the transition between 593 formation linear flow and compound linear flow is triggered by fracture inter-594 ference which causes a change of regime in the recovery rate. The formation 595 linear flow and the compound linear flow are determined by the fracture ge-596 ometry and fracture interference. Fig. 13 shows that the transition between 597 the formation linear flow and the compound linear flow happens at around 598 a time equal to τ (i.e. scaled time = 1). According to Freeman et al. (2013), 599 this change in flow regime will be matched by a change in recovery rate 600 regime. Fig. 14 locates this regime change in a plot showing the recovery 601



Figure 13: Left: formation linear flow, Centre: compound linear flow, Right: elliptical flow

rate vs. scaled time. This can be linked back to the work of Patzek et al. 602 (2013) and the two-regime flow analysed in Section 3.1.1. For $\tau < 1$, where 603 the recovery factor is proportional to the square root of scaled time, the 604 pressure contour does not show fracture interference. Therefore the square 605 root regime of the recovery factor can be associated with the absence of in-606 terference between the fractures (i.e. formation linear flow in the pressure 607 contours). The transition from formation linear flow to compound linear flow 608 around the fracture triggers the regime change in recovery rate at a scaled 609 time of 1.0. After fracture interference, the profile of the flow is expected to 610 be affected by the global geometry of the fracture network and the recovery 611 rate turns into exponential decay (Patzek et al. (2013)) if the fracture net-612 work is optimized for recovery, or a different profile depending on the global 613 characteristics of the fracture. In this second stage, the interaction with the 614



Figure 14: Recovery rate versus time, with the regime change highlighted at scaled t=1

reservoir confinement may also play an important role on the evolution of the shale flow. This will be further investigated in Section 3.3.

617 3.2. Diffusion Behaviour

Although shale gas flow is often described as a diffusion phenomenon (Patzek et al. (2013)), the governing equation (see Eq. 13) is not a pure diffusion equation because of the two extra terms appearing on the right hand side. In order to investigate the contribution of these two terms to the shale flow, results obtained in Section 3.1 for Case 1 (see Table 1) will be compared with results from a reduced model, where only the diffusion term in Eq. 13 is retained (for this test, PM4 was utilized):

$$\frac{\partial P}{\partial t} = \nabla \cdot \left(\frac{k}{\phi \mu C_g} \nabla P\right) \tag{24}$$

This equation is quite simple to implement and solve and can be viewed as a simplified model of the shale gas flow.

Comparisons between the solution obtained with the complete model 627 (Eq. 13, already discussed in Section 3.1) and the diffusion-only model (Eq. 24) 628 are shown in Fig. 15 where the logarithmic plot of the recovery factor and 629 the recovery rate vs. time are reported. It is possible to note that the use 630 of Eq. 24 leads to an overestimation of the recovery rate, and therefore an 631 overestimation of the recovery factor, compared to the complete model. This 632 means that the second and third terms on the right hand side of Eq. 13 have 633 the effect of reducing the diffusion mass flow rate. 634

⁶³⁵ Considering the depletion time, the difference between the two cases is ⁶³⁶ significant and this suggests that Eq. 24 cannot be used to model shale gas



(a) Logarithmic plot of the recovery factor (b) Logarithmic plot of the recovery rate vs. vs. time.

Figure 15: Comparison between the shale gas behaviour predicted by the complete model (Eq. 13) and the diffusion-only model (Eq. 24).

when accuracy is a critical factor. However, the trends in Fig. 15 show that the solution of Eq. 24 still preserves the two-regime flow. Therefore, although the additional terms in the complete model have an important impact on the mass flow rate, the physical behaviour seems dominated by diffusion.

The results in this section show that the flow of natural gas in shale is indeed a diffusion-dominated phenomenon. A diffusion equation can properly model the two-regime behaviour, but gives very different predictions of quantities relevant for practical purposes, such as the recovery factor and the recovery rate, compared to the complete model.

646 3.3. Influence of the geometry

Natural gas flow in shale is known to be strongly influenced by the fracture 647 network geometry (Patzek et al. (2013)). In order to further investigate this 648 aspect, four geometries with the same fracture network but with varying 649 reservoir sizes were solved. In all the cases the reservoir has the shape of a 650 parallelepiped with the same area of the cross section but different lengths, 651 as schematically shown in Fig. 16 and detailed in Table 3. Simulations with 652 variations of the other dimensions of the reservoir (for example the width) 653 were also performed (refer to Appendix A), leading to the same conclusions. 654 The results in Fig. 17 show that the recovery rate and the recovery factor 655 are the same for all geometries. Therefore it is possible to conclude that the 656

flow behaviour is determined by the fracture network, regardless of the dimension of the domain. Furthermore, Fig. 17 shows that all four geometries



Figure 16: Schematic of the cases considered for the sensitivity analysis to the reservoir dimension.

Table 3: Geometrical properties of the geometries used to investigate the effect of fracture network

Geometry	Reservoir Length	Reservoir Height	Reservoir Width
Geometry 1	$5 \mathrm{m}$	$5 \mathrm{m}$	$5 \mathrm{m}$
Geometry 2	$7 \mathrm{m}$	$5 \mathrm{m}$	$5 \mathrm{m}$
Geometry 3	9 m	$5 \mathrm{m}$	$5 \mathrm{m}$
Geometry 4	11 m	5 m	5 m

produce the same amount of gas after a given time is elapsed. This means 659 that, regardless of size, early shale gas behaviour is set by the fracture net-660 work. Only in the last stages of the depletion, when the flow interacts with 661 the boundary walls, the reservoir shape and dimension can affect the shale 662 production. In other words, the recovery rate is mainly dependent on the 663 fracture geometry, until boundary conditions of the reservoir come into effect. 664 This further validates the solver, as this behaviour is expected and agreed 665 upon in literature, as already discussed in Patzek et al. (2013); Freeman et al. 666 (2013).667



(a) Logarithmic plot of recovery rate vs. (b) Logarithmic plot of recovery vs. scaled scaled time time

Figure 17: Sensitivity analysis to the dimension of the reservoir.

668 3.4. Complex Geometry

As stated in Section 1, one of the main properties of shale gas reservoirs, 669 is the complexity of the fracture geometry. Since one of the main aims of this 670 work is to present a three-dimensional CFD solver able to solve very complex 671 fracture networks, it would be adequate to show the capability of the solver 672 to predict the shale flow in a more realistic fracture geometry. The geometry 673 was confined inside a block of matrix whose dimensions are $0.5 \times 0.5 \times 0.1$ m³. 674 and can be seen in Fig. 18. The permeability model PM3 (see Table 2) was 675 used to generate the results. Due to the complex geometry, in this case the 676 domain was discretized by means of a tetrahedral mesh generated using the 677 software ICEM, part of the ANSYS package. A time sequence of the pressure 678 and permeability distributions in the domain, is shown in Fig. 19. 679

It is interesting to note how in complex fracture geometries, the inter-680 action between the different fractures happens at different times being con-681 trolled by the inter-distance between the various fracture elements. As shown 682 in Fig. 19, in the region where two fracture elements are very close to each 683 other the pressure is quite low (higher local depletion) whereas where the 684 distance between the elements is bigger, the higher level of pressure indi-685 cates that a larger amount of shale gas is still present in that region. The 686 three-dimensional solver presented here is able to capture all these features 687 and solving in detail the shale flow around the fracture and, in principle, 688 the solution can also be used to calibrate low-order analytical models. For 689 the sake of completeness, the global recovery factor and the recovery rate 690 are reported in Fig. 20. The maximum recovery factor achieved in this case 691



Figure 18: Fracture geometry of the case presented in Section. 3.4

(see Fig. 20(b)) is around 62%. This is due to the outlet boundary condition set to 5 MPa, well above atmospheric pressure, which does not allow the complete depletion of the reservoir.

695 3.5. Dual Zone Solver

In principle, the mathematical model describing the shale behaviour can 696 be used to study the shale flow in both the matrix and the fracture. Keeping 697 in mind that the shale matrix and the fracture network vary greatly in perme-698 ability and porosity, the domain can be decomposed into two sub-domains, 699 corresponding to the matrix and the fracture respectively, where different 700 properties are assigned. This is the principle behind the dual zone solver 701 implemented in this work (see Section 2.3) where the governing equation of 702 the single zone solver is applied to both the matrix and the fracture and 703 the interaction between the two regions is imposed through specific coupling 704 conditions at the common interface. In order to distinguish between the two 705 regions, specific values of permeability and porosity should be assigned, con-706 sistent with the nature of the matrix and the fracture. With the main aim of 707 showing the capability of this approach, the dual zone solver has been used 708 to investigate the simple test case shown in Fig. 21. Although the solver 700 can be applied to any kind of geometry, as the ones used for the single zone 710 solver, this case was chosen for the very simple shape of the interface which 711 facilitates the meshing of the two domains (a one-to-one correspondence of 712 the faces at the interface is required in the current implementation) and at 713 the same time reduces the computational cost. The zone parameters used in 714



Figure 19: Pressure and permeability distribution vs time, in a complex fracture geometry.

the present investigation are detailed in Table 4. This model should not be 715 confused with the well known dual porosity model used to represent fractured 716 porous media, as already discussed in Section 2.3. The model presented here 717 does not require any transformation of the physical domain, and treats both 718 regions as completely separate. As a result, a porosity value of 33% assigned 719 to the fracture in Table 4 represents the porous space within the fracture 720 only, and does not represent the volume of the fracture with respect to the 721 whole fractured domain. In addition, since the fracture has a large aperture 722 compared to the shale matrix which has nanopores, a constant permeability 723 (PM1) was assigned to the fracture, whereas for the matrix both constant 724



Figure 20: Recovery Rate and Recovery Factor of the complex realistic geometry case.

Table 4: Properties of the matrix and the fracture for the case studied with the dual zone solver.

Property	Matrix	Fracture
Porosity	9%	33%
Permeability	PM1, $k = 5 \times 10^{-19} \text{ m}^2(506nD)$, or PM3	PM1, $k = 5 \times 10^{-15} \text{ m}^2 (1.013 \text{ mD})$
Initial Pore Pressure	35 MPa	35 MPa
Governing Equation	Eq. 13	Eq. 13
Common Boundary Condition	Dirichlet BC	Neumann BC
Confinement Boundary condition	Neumann zero gradient (wall)	Neumann zero gradient (wall)
Outlet	-not applicable-	Dirichlet BC (fixed value) 3MPa

permeability (PM1) and apparent permeability function (PM3) were tested,
as also summarized in Table 4.

Before looking at the results, it is important to note that the fracture 727 is in direct contact with the low pressure outlet boundary while the matrix 728 is interfaced with the fracture which is at the same initial pressure of the 729 matrix. Furthermore, the fracture permeability is $5 \times 10^{-15} \text{ m}^2$ (1.013 mD) 730 compared to 1×10^{-19} m² (101 nD) for the matrix, at 35 MPa. Therefore, 731 the fracture is expected to deplete first and at a faster rate compared to 732 the matrix or, in other words, the pressure in the fracture is expected to 733 balance the outlet pressure of 3.0 MPa long before the matrix. This is shown 734 in Fig. 22, where the pressure field in the case of constant permeability for 735 both the matrix and the fracture are reported. After 5 s the highest pressure 736 existing in the fracture is around 3.1 MPa, whereas a significant volume of 737 the matrix has still a pressure higher than 34.0 MPa, although the initial 738 pressure of both the fracture and the matrix was the same (35.0 MPa, see 739 Table 4), indicating that the fracture is almost depleted whereas the matrix 740





Figure 21: Schematic of the case studied with the dual zone solver.

Figure 22: Pressure field in the cross section at different times for the case investigated with the dual zone solver.

still contains the most of the initial shale gas.



Figure 23: Darcy velocity field in the cross section at different times for the case investigated with the dual solver.

It is also interesting to analyse the Darcy velocity shown in Fig. 23. Con-741 sistent with the time evolution of the pressure, the fracture Darcy velocity at 742 the interface with the outlet boundary decreases from 128 mm/s at t = 1 s 743 to about 1 mm/s at t = 5 s, whereas values lower than 0.5 mm/s are ob-744 served at the fracture/matrix interface throughout the transient indicating 745 that the fracture depletes faster than the matrix. Reminding that the Darcy 746 velocity in each region is proportional to the permeability and the pressure 747 gradient (see Eq. 2), the observed behaviour can be related to the time evo-748 lution of the pressure as well as the difference in permeability between the 749

two zones (the fracture permeability is four orders of magnitude larger than 750 the matrix permeability). At early times the pressure gradient at the frac-751 ture/outlet interface is very high and then decreases leading to a decrease 752 of the Darcy velocity, whereas pressure gradients at the fracture/matrix in-753 terface are generally low during the whole initial transient causing the lower 754 levels of velocity observed at the common interface. Looking more in detail 755 at the transient behaviour of the Darcy velocity at the common interface, it 756 is interesting to note that, as shown in Fig. 23, the velocity increases from 757 0.298 mm/s at t = 1 s to 0.37 mm/s at t = 3 s and then decreases back 758 to 0.329 mm/s at t = 5 s. Such behaviour can be explained on the basis 759 of the time evolution of the pressure gradient. Since the initial pressure in 760 the two domains, the fracture and the matrix, is the same, at early times 761 the pressure gradient at the interface is very small. However, as the fracture 762 starts to deplete this pressure gradient starts to increase. Owing to the high 763 permeability of the fracture network, the pressure in the fracture drops faster 764 than the pressure in the matrix which has a permeability four orders of mag-765 nitude smaller. This fast drop in fracture pressure coupled with a slow drop 766 in matrix pressure, causes the pressure gradient at the boundary in between 767 the two zones to increase rapidly, generating an increase of the velocity. After 768 that, as the pressure in the matrix starts to decrease gradually, the velocity 769 at the interface starts to decrease as well until the complete depletion. 770

Since the coupling conditions at the common interface impose the same 771 pressure and the same mass flow rate (see Section 2.3 for details), both the 772 pressure and the Darcy velocity at the two sides of the interface should be 773 the same. This is clearly shown in Figs. 22 and 23, thus verifying that the 774 coupling at the boundary is correctly working. This also means that, because 775 of the different values of permeability, the pressure gradient on the matrix 776 side is higher than the one on the fracture side. This has implications for the 777 generation of the mesh. In order to properly resolve the pressure gradient, a 778 higher resolution is generally required on the matrix side of the interface in 779 order to proper resolve 780

The different behaviour of the Darcy velocity at the outlet boundary and at the fracture/matrix interface has a direct impact on the recovery rate of the two zones, which is directly related to the velocity field. Figures 24(a)-(d) show the recovery factor and recovery rate of the matrix and the fracture, considered as two distinct domains. The recovery rate and the recovery factor of the fracture qualitatively resembles the two regime flow (diffusion dominated) whereas the recovery rate of the matrix (flow rate exiting the



Figure 24: Recovery rate and recovery factor of the matrix, fracture and matrix and fracture combined predicted by the dual zone solver with constant permeability for both the fracture and the matrix.

matrix into the fracture zone, Fig. 24(a)) initially increases followed by a decrease with the typical behaviour observed with the single zone solver (the fast drop in recovery rate is unique to shale flow). This is due the previously discussed behaviour of the Darcy velocity at the fracture/matrix interface. Results show a great deal of disparity between the behaviour of flow within the matrix and the fracture, but the overall result of the two domains combined still qualitatively complies with the two regime flow as can be seen in Figs. 24(e)-(f), which represent the recovery factor and recovery rate of the matrix and fracture domains combined as one whole domain.

Results presented so far were obtained with a constant permeability for 797 both the matrix and the fracture. However, different permeability models 798 can be used. For example, a more physically consistent simulation can be 799 performed using an apparent permeability for the matrix, in order to include 800 Knudsen effects. The recovery rate and recovery factor of matrix, fracture 801 and the whole domain (fracture and matrix combined) obtained by assign-802 ing the apparent permeability to the matrix are shown in Fig. 25. Results 803 are qualitatively similar to the one obtained for the case with constant per-804 meability (the same applies to the pressure and velocity fields) with some 805 differences due to the change of permeability with pressure (see Fig. 3(b)). 806

At the very beginning of the simulation, where the pressure is very close to the initial condition, the apparent permeability is lower than 10^{-19} m²(101 nD) and the depletion of the matrix is slower compared to the previous case. The recovery rate should improve during the last stages where because of the smaller pressures the apparent permeability increases.

Results presented in this section provide a fresh attempt at modelling 812 shale flow behaviour, where the coupled behaviour of the fracture and the 813 matrix can be analysed giving more insight into the processes affecting shale 814 gas flow. The flexibility of the code with respect to the physical proper-815 ties (e.g. permeability model) of the different domains allows us to model 816 the fracture and the matrix with the models and parameters that are more 817 representative of the actual physical behaviour. It should be noted that 818 this dual zone approach can be very expensive (in terms of computational 819 cost) for cases characterized by a very large and intricate fracture network. 820 However, the detailed results that can be obtained with this approach can 821 be exploited to assess and possibly calibrate low-order models for shale gas 822 flow. 823



Figure 25: Recovery rate and recovery factor of the matrix, fracture and matrix and fracture combined predicted by the dual zone solver with apparent permeability for the matrix and constant permeability for the fracture.

824 4. Conclusion

This study presented a three dimensional CFD solver to simulate shale gas flow in porous media utilizing the OpenFOAM framework. A tailored

governing equation that does not require the use of pseudo pressures, because 827 the numerical solver implements the gas properties as functions of pressure, 828 was utilized. The proposed approach allows using different relations for the 829 properties on the basis of the case under investigation or the choice of the 830 user. First, the solver was validated against the findings of Patzek et al. 831 (2013) and Freeman et al. (2013). It was found that the recovery rate and 832 the recovery factor match a two regime flow. The rate of increase in recovery 833 factor, κ , depends on the fracture geometry, permeability, and initial con-834 ditions. Then, four permeability models were implemented to account for 835 stress effects and Knudsen and slip flow. The results confirmed the domi-836 nance of the diffusion aspect on shale flow, as the results were comparable 837 and the trends were similar between the governing equation and a diffusion 838 equation. In addition, it was noted that the fracture network geometry im-839 poses the recovery rate. The flow was indistinguishable, even after fracture 840 interference, for four reservoirs with the same fracture network but with dif-841 ferent reservoir dimensions. Finally, an extension was developed based on 842 the single solver, named the dual solver, drawing inspiration from the dual 843 porosity/dual permeability models as well as previous heat transfer models. 844 The physical geometry is preserved and directly solved, without any trans-845 formation. The dual solver treats the matrix and the fracture network as 846 two separate zones, each with its own governing equations and parameters. 847 The recovery rate of the whole domain qualitatively adhered to the diffu-848 sion dominated two regime flow. Different permeability models were also 849 implemented. 850

⁸⁵¹ Appendix A. Additional Results

As noted in Sections 2.4.1 and 2.4.3, additional results were produced for Case 2, using the viscosity and permeability relations given by Eqs. B.1 and B.2 in order to assess the effect of using different viscosity and compressibility factor relations proposed in literature. This further points out the flexibility of the proposed approach, which allows implementing any gas property relation, as previously discussed in Section 2.4.

Fig. A.26 shows that, for the investigated case, recovery factor and recovery rate still adhere to the two regime flow described in Section 3.1.1. When comparing Fig. A.26 with Fig. 9(a,c) and Fig. 11(a,c), the variation in results between using Eqs. 17, 20 and Eqs. B.1, B.2 is minor, and the same slopes are used to match the results.



Figure A.26: Recovery rate and recovery factor versus scaled time for Case 2 predicted using the equation of state and the viscosity relationships from Jarrahian et al. (2015); Jarrahian and Heidaryan (2014) (Eq. B.1 and Eq. B.2, with curve matching.)

Fig. A.27 shows the geometry of the case referred to in Section 3.3, when the change in width is tested. Fig. A.28 indicates that the results are the similar to that of varying length. The same conclusion can be made; the flow behaviour is determined by the fracture network.



Figure A.27: Schematic of the extra cases considered for the sensitivity analysis to the reservoir dimension.



(a) Logarithmic plot of recovery rate vs. (b) Logarithmic plot of recovery vs. scaled scaled time time

Figure A.28: Sensitivity analysis to the dimension of the reservoir.

⁸⁶⁷ Appendix B. Additional Equations

Appendix B includes the equations referred to, but not included in the body of this paper.

$$z = \frac{PV}{RT} = 1 + \frac{1}{V} \left(b - \frac{a\beta}{RT} \right) + \frac{1}{V^2} b \left(b + \frac{a\beta}{RT} \right)$$
$$\beta = \beta_1 + \beta_2 Ln P_{pr} + \frac{\beta_3}{T_{pr}} + 4\beta_4 Ln^2 P_{pr} + \frac{\beta_5}{T_{pr}^2} + \frac{\beta_6 Ln P_{pr}}{T_{pr}}$$
$$a = 0.49694 \frac{(RT_{pC})^2}{P_{pC}}$$
$$b = 0.09012 \frac{RT_{pC}}{P_{pC}}$$

(R 1)

where β_1 , β_2 , β_3 , β_4 , β_5 , β_6 , T_{pr} , P_{pC} , T_{pC} are provided in Jarrahian and Heidaryan (2014).

$$\mu_{g} = 1 + \left(A_{1} + \frac{A_{2}}{T_{pr}} + \frac{A_{3}}{T_{pr}^{3}}\right)\rho_{R} + \left(A_{4} + \frac{A_{5}}{T_{pr}}\right)\rho_{R}^{2} + \left(\frac{A_{5}A_{6}}{T_{pr}}\right)\rho_{R}^{5} + \left(\frac{A_{7}}{T_{pr}^{3}}\right)\rho_{R}^{2}(1 + s\rho_{R}^{2})Exp(-A_{8}\rho_{R}^{2})$$

$$\mu_{atm} = \frac{C_{1}T_{pr}^{C_{2}} + C_{3}Exp(C_{4}T_{pr}) + C_{5}Exp(C_{6}T_{pr}) + C_{7}}{\zeta} + \Delta\mu(H_{2})$$

$$\rho_{R} = \frac{P_{pr}}{(B_{1} + B_{2}\gamma_{g})ZT_{pr}}$$

$$\zeta = \frac{T_{pC}}{M_{w}^{3}P_{pC}^{4}}$$
(B.2)

where A_1 , A_2 , A_3 , A_4 , A_5 , A_6 , A_7 , A_8 , B_1 , B_2 , C_1 , C_2 , C_3 , C_4 , C_5 , C_6 , C_7 , T_{pr} , P_{pr} , P_{pC} , T_{pC} , and $\Delta \mu(H_2)$ are provided in Jarrahian et al. (2015).

872 Appendix C. Nomenclature

873 Symbols

A	Surface Area, m^2
C_q	Gas Compressibility, 1/Pa
C_r	Reduced Gas Compressibility
d	Fracture Spacing, m
h	Elevation, m
k	Absolute Permeability, m^2
m	Recovered gas mass, kg
M	Initial gas mass, kg
P	Pressure, Pa
P_{cr}	Critical Pressure, Pa
PM	Permeability Model
RF	Recovery Factor
t	Time, s
\tilde{t}	Scaled Time
T_{cr}	Critical Temperature, K

u	Darcy Velocity, m/s
M_w	Molar Mass, kg/kmol
r	Pore Radius, m
R	Universal Gas Constant, 8.314 J/(mol.K)
z	Compressibility Factor
α	Tangential Momentum Accommodation Coefficient
ϕ	Porosity
μ	Viscosity, Pa.s
ρ	Density, kg/m^3
τ	Characteristic Interference Time, s

874 Subscript

a	Apparent
avg	Average
f	Fracture
m	Matrix
n	Normal component

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