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1 highlights

- We analyse advective and conductive heat transport in rock fractures,
 coupled to heat conduction in the matrix
- Flow channeling strongly impacts heat transport through fractures and fracture-matrix heat exchange
- The thermal behavior at the fracture scale can be predicted from the fracture's effective hydraulic transmissivity

Journal Prevent

8	Heat transport by flow through rough rock fractures:
9	a numerical investigation
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15 Abstract

Fracture surface topography exhibits long-range spatial correlations resulting in a heterogeneous aperture field. This leads to the formation, within fracture planes, of preferential flow channels controlling flow and transport processes. By means of a 3-D heat transport model coupled with a 2-D fracture flow model based on the lubrification approximation (i.e., local cubic law), we investigate how the statistical parameters determining spatial aperture variations in individual fractures control the heat exchange at the fluid/rock interface and heat transport by flow. Ensemble statistics over fracture realizations provide insights into the main hydraulic and geometrical parameters controlling the hydraulic and thermal behaviour of rough fractures. Similarly to the rough fracture's hydraulic behaviour, we find that its heat transport behaviour deviates from the conventional parallel plate fracture model with increasing fracture closure and/or decreasing correlation length. We demonstrate that the advancement of the thermal front is typically slower in rough fractures compared to smooth fractures having the same mechanical aperture. In contrast with previous studies that neglect temporal and spatial temperature variations in the rock matrix, we find that the thermal behavior of a rough-walled fracture can, under field-relevant conditions, be predicted from a parallel plate model with an aperture equal to the rough fracture's effective hydraulic aperture. This greatly simplifies the prediction of possible reservoir thermal behavior when using field measurable quantities and hydrological modeling.

¹⁶ Keywords: Fracture, Roughness, Heat exchange, Flow channeling

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17 1. Introduction

Heat transport in fractured media is often considered in hydrogeological 18 studies, for instance, when inferring hydraulic parameters by fitting heat 19 transfer equations to thermal data. Heat carried by groundwater serves 20 as a tracer that can be used to quantify flow through fractures [Ge, 1998; 21 Read et al., 2013, to characterize fracture network connectivity [Silliman 22 and Robinson, 1989; Klepikova et al., 2011, 2014] and to constrain regional 23 scale flow patterns [Anderson, 2005; Saar, 2010]. Understanding heat trans-24 port in fractured media is a prerequisite for studying hydrothermal flows 25 [Fairley, 2009; Malkovsky and Magri, 2016]. Moreover, characterizing heat 26 transport processes in the subsurface is essential for numerous industrial ap-27 plications. For instance, heat transfer is critical when assessing heat storage 28 in the ground [Lanahan and Tabares-Velasco, 2017; de La Bernardie et al., 29 2019] and near-field thermal effects in the context of radioactive waste dis-30 posal [Zhang et al., 2017]. Knowledge of thermal transport is also necessary 31 to maximize the efficiency and sustainability of geothermal systems [Kolditz 32 and Clauser, 1998; Martinez et al., 2014; Shortall et al., 2015; Guo et al., 33 2016; Vik et al., 2018; Patterson and Driesner, 2020]. 34

Heat transport in fractured media has predominantly been addressed us-35 ing simplified conceptual fracture models. For example, most fracture net-36 work models used for geothermal investigations assume a 1-D linear flow ge-37 ometry [Pruess and Doughty, 2010], or consider fractures as parallel-plate sys-38 tems with a constant aperture [Gringarten et al., 1975; Kolditz and Clauser, 39 1998; Kocabas, 2005; Jung and Pruess, 2012; Zhou et al., 2017; Vik et al., 40 2018]. Hydrothermal studies generally represent faults as tabular bodies 41 of internally homogeneous properties or as 2-D discontinuities that juxta-42 pose hydrogeologic units of differing properties [e.g. Malkovsky and Magri, 43 2016. While it is common practice to neglect fracture heterogeneity, the 44 consequences of such simplifications in terms of predictability remain poorly 45 understood [Klepikova et al., 2016; de La Bernardie et al., 2019]. 46

The fracturing process itself, as well as post-fracturing processes such as geological stress and strain, chemical dissolution, precipitation and erosion, may result in complex fracture-wall surface geometries. At the scale of a single fracture, fracture wall roughness exhibits long range spatial correlations that induce a heterogeneous aperture field [Brown, 1987; Johns et al., 1993; Candela et al., 2012], thus, promoting strongly heterogeneous flow path distributions and preferential flow channels within fracture planes [e.g. Tsang

and Tsang, 1987: Méheust and Schmittbuhl, 2000: Méheust and Schmittbuhl, 54 2001]. Numerous studies have shown that fracture roughness has a remark-55 ably strong impact on fluid flow and, as a consequence, on solute and particle 56 transport through single fractures. Studies of flow and solute transport in 57 rough-walled fractures include both theoretical and numerical studies [e.g 58 Ge, 1997; Méheust and Schmittbuhl, 2001, 2003; Boutt et al., 2006; Carde-59 nas et al., 2009; Wang and Cardenas, 2014, 2017; Yang et al., 2019; Yoon 60 and Kang, 2021, as well as laboratory experiments [e.g. Plouraboué et al., 61 2000; Méheust and Schmittbuhl, 2000; Detwiler et al., 2000; Boschan et al., 62 2007, 2008; Ishibashi et al., 2015]. 63

More recently, flow channeling in fractured media has been recognized as 64 a critical control on heat transport as well [e.g Geiger and Emmanuel, 2010; 65 Luo et al., 2016]. Based on numerical simulations of flow and heat transport, 66 Neuville et al. [2010b] found that the heat exchange between the rock and the 67 fluid is either enhanced or decreased in rough fractures compared to smooth 68 fractures with equivalent mechanical apertures, depending on the fracture's 69 morphology and aspect ratio. They concluded that because of the presence 70 of larger flow velocities, leading to reduced transit times in the channeled 71 areas, the heat exchange is generally less efficient in fractures with variable 72 apertures compared to smooth fractures (the so-called parallel plate) with the 73 same hydraulic aperture. The authors applied their modeling approach to 74 the geothermal reservoir of Soultz-sous-Forêts, France, leading to predictions 75 of decreased thermal exchanges in rough fractures compared to smooth ones 76 having identical hydraulic transmissivities [Neuville et al., 2010a]. In their 77 modelling studies, Neuville et al. [2010b,a, 2011] neglected temporal and 78 spatial temperature variations within the rock matrix. 79

Neuville et al. [2013] moved beyond the assumption of constant matrix 80 temperatures and demonstrated that the hydrothermal behavior within a 81 fracture is heavily influenced by fracture-matrix heat exchange processes. In 82 their study, the Navier-Stokes equations and advection-diffusion equations 83 were solved in a simple 3-D model of a fracture consisting of flat parallel 84 walls perturbed by a single sharp asperity [Neuville et al., 2013]. More re-85 cently, using a 3-D numerical model in which the flow in the fracture is 86 described by the Reynolds equation, Fox et al. [2015] offered practical un-87 derstanding of the effects that fracture aperture variations have on heat pro-88 duction in geothermal reservoirs. Notably, Fox et al. [2015] demonstrated 89 that the thermal exchanges between the fluid flowing within a rough-walled 90 fracture and the surrounding matrix are reduced in comparison to planar 91

surfaces, because flow channeling reduces the contact area over which heat 92 conductive transfer takes place. They conclude that, as a consequence, frac-93 ture aperture variations generally have a negative impact on the thermal 94 performance of geothermal reservoirs. More recently, from theoretical and 95 numerical analyses of heat transfer in geometrically simple 3-D conceptual 96 models of fractures, Klepikova et al. [2016] demonstrated that flow channeling 97 locally enhances heat diffusion rates because a channel (cylindrical conduit) 98 is more efficient in exchanging heat between a fracture and the matrix than a 99 planar fracture of equivalent surface. Regardless of the different underlying 100 assumptions, these results reveal that two opposing effects related to flow 101 channeling impact fracture-matrix heat exchange at the fracture scale. On 102 the one hand, heat transfer is locally enhanced by increasing the dimension-103 ality of the diffusive flux [Klepikova et al., 2016]; on the other hand, heat 104 transfer is reduced by decreasing the effective contact area [Fox et al., 2015; 105 Guo et al., 2016]. Consequently, it is necessary to jointly quantify the un-106 derlying mechanisms using high-fidelity physics and modelling, in order to 107 understand which of those opposing effects is dominant, and under which 108 conditions. 109

The results of recent field experiments also call for the development of 110 numerical modelling that considers flow channeling within individual frac-111 tures. Heat tracer experiments have been conducted recently, for example, 112 at the experimental site of Ploemeur, France (H+ observatory network) [Read 113 et al., 2013; Klepikova et al., 2016; de La Bernardie et al., 2019], in a field 114 site in Altona, NY [Hawkins et al., 2017] and at the Grimsel Test Site (GTS), 115 Switzerland [Doetsch et al., 2018]. These in situ experiments have demon-116 strated that, due to the signature of fracture heterogeneity on heat transfer 117 processes, predictions based on the classical parallel plate fracture model dif-118 fer significantly from field observations in terms of the first arrival time, the 119 maximum amplitude and the tailing of the thermal breakthrough. 120

We present a numerical study in which the fracture is described in two 121 dimensions (2-D) and the impermeable rock matrix in three dimensions (3-122 D). The flow in the fracture is described by the Reynolds equation, that is, 123 assuming that the lubrication approximation (and hence, the local cubic law) 124 is valid, while heat transport is described by the advection-diffusion equation 125 in 2-D in the fracture plane, and in 3-D in the matrix. This formulation 126 allows us to investigate heat transport along the fracture plane and in the 127 matrix, as well as heat exchange between them, while allowing for much 128 faster numerical simulations than with a 3-D discretization of the fracture. 129

We simulate 20 different rough topographies with a Hurst exponent $\zeta = 0.8$, 130 with aperture closures $\gamma/d_{\rm m}$ varying from 0.001 to 0.6 over a wide range 131 of mean fracture apertures, and with four different values of the mismatch 132 scale $L/L_c = 1, 2, 4, 16$. More precisely, we investigate how these properties 133 impact heat exchange at the fluid/rock interface and heat transport along a 134 fracture, in terms of the mean behavior among 20 fractures having such a 135 geometry. We address how flow heterogeneity within the fracture affects the 136 macroscopic properties (i.e., the hydraulic transmissivity, the velocity of the 137 thermal front, and its width) ultimately governing the efficiency of the fluid 138 mass and heat transport through the fracture. 139

Compared to previous studies considering simplified fracture geometry 140 [Gringarten et al., 1975; Kocabas, 2005; Pruess and Doughty, 2010; Jung 141 and Pruess, 2012; Neuville et al., 2013; Klepikova et al., 2016; Zhou et al., 142 2017] and/or a simplified heat transfer model [Neuville et al., 2010b,a, 2011], 143 the developed numerical model of flow and heat transport considers simul-144 taneously heat conduction in the matrix and in the fracture, as well as heat 145 advection coupled to flow channeling in the fracture. Transient alteration of 146 the fracture's geometry due to thermo-hydro-mechanical-chemical (THMC) 147 coupling [Tsang, 1991; Taron and Elsworth, 2009; Pandey et al., 2014; Guo 148 et al., 2016; Salimzadeh and Nick, 2019; Patterson and Driesner, 2020] are 149 not considered as such effects are mainly relevant for very sharp temperature 150 contrasts and typically act over time scales of months or years. Compared to 151 recent works investigating heat transfer within rock samples [Luo et al., 2017; 152 Chen and Zhao, 2020, our modelling results allow evaluating the impact of 153 the (statistical) geometrical properties of a single geological fracture on heat 154 transfer and to determine the key controlling parameters. Ultimately, this 155 work aims at providing improved parameterizations and guidance for effec-156 tive low-dimensional fracture models. The presented results also advance our 157 understanding of how fracture heterogeneity control the efficiency of diffusive 158 exchange processes at the fracture scale. 159

This paper is organized as follows. Section 2 describes the physical con-160 ceptualization and the implemented numerical approach. The numerical re-161 sults are presented in Section 3, where we first describe the results for a given 162 aperture-field realizations, and then present the general trends that are ob-163 served when considering large sets of synthetic fracture fields. The relevance 164 of our models to practical configurations and applications is discussed in Sec-165 tion 4. Finally, Section 5 concludes with a summary of the most important 166 findings, and outlines possible future developments. 167

¹⁶⁸ 2. Methods

To investigate the sensitivity of the hydrothermal behavior of a roughwalled fracture embedded in a homogeneous rock matrix to statistical fracture aperture properties, we develop a numerical model of flow and heat transport. We first present the self-affine aperture fracture model. Then, we develop a numerical model of flow and heat transport using the finite element-based software COMSOL Multiphysics[®] [COMSOL Multiphysics User's Guide, Version 5.4., 2018], as detailed in the following.

176 2.1. Roughness of fracture aperture

We consider fractures whose projection on the mean fracture plane is 177 square and of lateral length L. Experimental studies carried out on cores 178 from natural joints [Brown et al., 1986] have shown that the two fracture walls 179 are self-affine, but are matched, that is they display identical topography 180 fluctuations, at scales larger than a critical length scale $L_{\rm c} \leq L$. This scale, 181 also denoted *mismatch scale*, is the upper limit to the self-affinity of the 182 aperture field. It is the only characteristic scale smaller than L available to 183 describe the aperture geometry, and is a property related to the regimes of 184 faulting (e.g., strike-slip, normal) and the history of the fracture (erosion, 185 dissolution, precipitation processes) which is independent of the fracture size 186 L [de Dreuzy et al., 2012]. 187

Using an algorithm adapted from Méheust and Schmittbuhl [2003], we 188 generate fracture aperture fields $d_{\rm fr}(x, y)$ with periodic boundary conditions 189 that are self-affine up to $L_{\rm c}$ and have a mechanical aperture $d_{\rm m}$ (i.e., the 190 distance between the mean planes of the fracture walls, which are parallel to 191 each other; if the walls are nowhere in contact, then the mechanical aperture 192 is the average value of $d_{\rm fr}(x, y)$, and standard deviation γ of the aperture field 193 over the entire fracture. In our model, the Hurst (or, roughness) exponent 194 has been chosen constant at $\zeta = 0.8$, a value observed for many natural and 195 artificial fracture surfaces [Schmittbuhl et al., 1993; Bouchaud, 1997; Renard 196 et al., 2013]. Each fracture is characterized by the fracture closure $\gamma/d_{\rm m}$, 197 which expresses the vertical extent of roughness relative to the fracture wall 198 separation. To keep a simple boundary geometry of the domain, we prevent 199 contact between fracture surfaces by only considering relatively small fracture 200 closures. Consequently, the mechanical aperture is also the mean aperture. 201 Due to stochastic variations, the mean aperture of the realizations deviates 202 slightly from the value specified when generating the field. Here and below, 203

 $d_{\rm m}$ refers to the actual mechanical apertures of each fracture realization, and the size of the fracture is fixed to L = 10 m. The grid size is 1024×1024 . Using different seeds of the random generator of the white noise used in the algorithm, it is possible to generate multiple independent self-affine aperture realizations with the same underlying statistical parameters. An example of a fracture aperture profile is shown in Figure 1b.

210 2.2. Hydrothermal modelling

211 2.2.1. Hydraulic flow

Flow within a fracture is modeled as a steady-state flow where viscous 212 forces dominate inertial effects, that is, at a low Reynolds number. Fur-213 thermore, we apply the lubrication approximation, according to which frac-214 ture walls have small local slopes [Zimmerman and Yeo, 2013]. Under these 215 assumptions, out-of-plane (i.e., along z) components of fluid flow become 216 negligible, and the velocity field is dominated by in-plane components. Con-217 sequently, the hydraulic flow through the fracture, q, defined as the integral 218 over the local fracture aperture of the fluid velocity \boldsymbol{u} , can be related to 219 local apertures through a local cubic law similar to the law used for smooth 220 (parallel plate) fractures [Méheust and Schmittbuhl, 2001; Zimmerman and 221 Yeo, 2013]: 222

$$\boldsymbol{q} = -\frac{d_{\rm fr}^3(x,y)}{12\eta} \boldsymbol{\nabla} P,\tag{1}$$

where P is the local pressure [Pa] and η is the fluid's dynamic viscosity [Pa 223 s]. P and q only depend on the two spatial coordinates that define the 224 fracture's mean plane, which will be simply denoted "fracture plane" in the 225 following. For quasi-parallel flows, the Reynolds number is generally defined 226 as $Re = U_{\text{charact}}(\rho_{\rm f} l_z^2)/(\eta l_{\rm h})$ [Méheust and Schmittbuhl, 2001; Neuville et al., 227 2011], where $\rho_{\rm f}$ is the fluid density [kg/m³], l_z and $l_{\rm h}$ denote estimates of the 228 vertical and horizontal scales of variation of the velocities [m], $U_{charact}$ is a 229 characteristic velocity which we choose equal to the maximum velocity within 230 a parallel plate fracture geometry of aperture $d_{\rm m}$, that is, $u_{\rm M} = \nabla P d_{\rm m}^2 / 8\eta$ 231 as estimated from the classical cubic law. In the particular case of a rough 232 fracture, one can consider $l_z = d_m$ and $l_h = L_c$, so Re can be expressed as 233

$$Re = u_{\rm M} \frac{\rho_{\rm f} d_{\rm m}^2}{\eta L_{\rm c}},\tag{2}$$

For the flow to remain linear in the fracture, the Reynolds numbers should be low, that is, Re < 1 [Oron and Berkowitz, 1998; Brush and Thomson, 2003; Lee et al., 2015].

Furthermore, we assume the fluid to be incompressible $(\nabla \cdot \boldsymbol{u} = 0)$, which implies that \boldsymbol{q} is also conservative: $\nabla \cdot \boldsymbol{q} = 0$ [Plouraboué et al., 2000]. Inserting the local cubic law (Equation (1)) in this conservation law yields the Reynolds equation:

$$\boldsymbol{\nabla} \cdot \left(d_{\mathrm{fr}}^3(x, y) \boldsymbol{\nabla} P \right) = 0. \tag{3}$$

As boundary conditions, we impose the pressure at the inlet (x = 0) and 241 outlet (x = L) of the fracture, resulting in a macroscopic pressure gradi-242 ent ∇P , and consider periodic boundary conditions at y = 0 and y = L. 243 The aperture field of the fracture also has periodic boundary conditions by 244 construction (i.e., apertures at x = L are identical to those at x = 0). 245 Although this condition is artificial, it is more appropriate than assigning 246 no-flow boundaries, which could restrict the flow, thus limiting the sensi-247 tivity to fracture properties [e.g. Odling, 1992; Oron and Berkowitz, 1998; 248 Méheust and Schmittbuhl, 2001]. The surrounding rock matrix is assumed 249 to be impermeable. An example of the hydraulic flow computed inside a 250 fracture's aperture field, a profile of which is shown in Figure 1b, is shown in 251 Figure 1a as black arrows. 252



Figure 1: (a) 3-D sketch of a fracture model. The x-axis is along the mean hydraulic flow, the y-axis is along the mean fracture plane and perpendicular to the x-axis, and the z-axis denotes the out-of-plane direction (with respect to the mean plane). Filled color represents the temperature anomaly after 1000 s of injection. The arrows represent the direction of the flow within the fracture with the arrow length proportional to the computed flow velocity. The fracture is embedded in a homogeneous and impermeable rock matrix. The horizontal extent of the fracture is 10 m×10 m. (b) The local fracture aperture d profile along y = 5 m (shown by yellow dashed line in (a)). The mean fracture aperture $d_{\rm m}$ is shown by the dashed line.

The permeability of a rough fracture depends both on the mean aperture and the geometry of the rock walls. The hydraulic aperture for a rough fracture is classically defined as the aperture of the parallel plate (i.e., smooth) fracture of identical transmissivity. It can thus be computed from the measured flux Q and imposed pressure gradient ΔP along the fracture [Tsang, 1992] as:

$$d_{\rm h} = \left(\frac{12\eta Q}{\Delta P}\right)^{\frac{1}{3}}.$$
 (4)

In the field, the hydraulic aperture can be assessed based on hydraulic transmissivity measurement obtained, for example, by pumping tests, while mechanical aperture can be assessed from roughness analysis on core material.

263 2.2.2. Heat transport

The 3-D finite element modeling tool COMSOL Multiphysics[®] allows 264 for straightforward coupling of fluid flow and heat transport. We consider 265 conductive and advective heat transport in the fracture, and heat conduction 266 in the surrounding rock matrix. Moreover, our modelling approach allows 267 avoiding 3-D discretization of a thin fracture domain, which would lead to 268 very large computational times when considering realistic ratios of the size 269 of the matrix along z to the mean fracture aperture. Figure 1a presents a 270 3-D sketch of our model with a fracture located within the x - y plane that 271 is surrounded by the impermeable rock matrix at |z| > 0. 272

We assume that fluid at a constant pressure and temperature of $T_{\rm inj}$ en-273 ters the fracture, initially at temperature T_{rock} , at the left model boundary 274 (x = 0), and flows in response to the imposed pressure gradient from left to 275 right. The rock temperature at the outer boundaries as well as the temper-276 ature at the fracture outlet are $T_{\rm rock}$. The injected fluid temperature is here 277 warmer $(T_{inj} > T_{rock})$ than the initial rock temperature, a scenario typically 278 encountered during hydrological investigations, in hydro-carbon recovery or 279 in nuclear waste leakage. In the following, we shall consider the relative 280 temperature deviation from the host rock's initial temperature (defined in 281 Eq. 10), so the results for the injection of a colder fluid $(T_{\rm inj} < T_{\rm rock})$, a 282 scenario typical of geothermal systems, would be exactly identical. 283

Several studies have found that heat conduction in the matrix in the direction parallel to the fracture has only a minor effect on the temperature distribution [e.g. Jung and Pruess, 2012]. We do consider horizontal conductive heat transport in the matrix, but assume that the conductive heat flux through the boundaries at x, y < 0 and at x, y > L can be neglected,

and hence we do not extend the rock matrix in these directions beyond the 289 fracture length. The thickness of the rock matrix layer D = 2 m was chosen 290 sufficiently large not to influence the temperature field within the fracture 291 during the simulation time. The boundary conditions for temperature at 292 the lateral boundaries of the fracture are periodic, similarly to those for 293 the aperture field and local flux field. We neglect natural convection by 294 temperature-induced bouyancy effects, that is, we consider that the fluid's 295 density is independent of its temperature. The heat transport in the system 296 can then be described as follows. 297

²⁹⁸ In the impermeable rock matrix:

$$\rho_{\rm r} C_{\rm p,r} \frac{\partial T}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{q}_{\rm r}^{(h)} = Q^{(h)}, \qquad (5)$$

 $_{\rm 299}~$ where the conductive heat flux is given by

$$\boldsymbol{q}_{\mathrm{r}}^{(h)} = -k_{\mathrm{r}} \boldsymbol{\nabla} T. \tag{6}$$

300 In the fracture:

$$d_{\rm fr}\rho_{\rm f}C_{\rm p,f}\frac{\partial T}{\partial t} + d_{\rm fr}\rho_{\rm f}C_{\rm p,f}\,\boldsymbol{u}\cdot\boldsymbol{\nabla}_{\rm t}T + \boldsymbol{\nabla}_{\rm t}\cdot\boldsymbol{q}_{\rm fr}^{(h)} = Q^{(h)},\tag{7}$$

 $_{301}$ where the conductive heat flux is given by

$$\boldsymbol{q}_{\rm fr}^{(h)} = -d_{\rm fr}k_{\rm f}\boldsymbol{\nabla}_{t}T.$$
(8)

Here $\nabla_{\rm t}$ denotes the gradient operator restricted to the fracture's tangential plane, ρ the density [kg/m³], $C_{\rm p}$ the heat capacity [J/kgK], k the thermal conductivity [W/mK], \boldsymbol{u} the local fluid velocity field [m/s], and the f, fr and r subscripts denote the fluid, fracture and rock, respectively.

The transport is characterized by the dimensionless thermal Péclet number Pe, which is the ratio between the characteristic times of heat diffusion/conduction and advection in the fracture [e.g. Ge, 1998; Gossler et al., 2019]:

$$Pe = \frac{u_{\rm M} d_{\rm m} \rho_{\rm f} C_{\rm p,f}}{k_{\rm r}}.$$
(9)

The numerical model relies on a 2-D discretization of the fracture plane and the 3-D discretization of the matrix domain. To capture with sufficient accuracy the relative variations of temperature, we imposed a finer mesh size around the fracture (~ 0.02 m), while the coarser elements (~ 0.2 m) are located near the outer boundaries of the rock matrix. We verified that refining the element size by a factor of 2 did not influence the resulting temperature field significantly (<0.1 %). Since we ignore thermo-hydro-mechanicalchemical (THMC) processes in this study (see Introduction and Discussion), all physical properties are assumed to be time-invariant.

For all the the computations done in this study, the pressure gradient was 319 chosen such that the Péclet number is Pe = 51. Such a high Péclet number 320 implies that heat advection in the fracture is much faster than heat con-321 duction in the matrix. The simulations are done at low Reynolds numbers, 322 the maximum Reynolds number being Re = 0.8 (for fracture apertures as 323 high as $d_{\rm m}=23$ mm), which is compatible with the lubrication approximation 324 (and hence, the local cubic law). Note, that while the definition of Péclet 325 and Reynolds numbers varies between studies, the range of velocities and 326 apertures studied herein is similar to those reported in previous works [e.g. 327 Neuville et al., 2013, 2011]. Here and below, thermal parameters are selected 328 to represent granite, the host formations of most deep geothermal projects 329 (Table 1). 330

Table 1: Chosen rock properties representative of granite. The thermal parameters are taken from Incropera and DeWitt [1996]; Klepikova et al. [2016] and Kant et al. [2017].

Parameter	Matrix, $_{\rm r}$	Water, $_{\rm f}$
Density ρ , kg/m ³	2500	1000
Thermal conductivity k , W/(m K)	0.59	3.5
Heat capacity $C_{\rm p}$, J/(kg K)	750	4189

331 3. Results

332 3.1. Hydraulic behaviour

In Figure 2a we present the ratio of hydraulic to mechanical apertures 333 $d_{\rm h}/d_{\rm m}$, as a function of the fracture closure $\gamma/d_{\rm m}$ for 20 families of fractures. 334 A family of fractures refers here to a set of fractures generated with the 335 same random seed, but with different fracture closure $\gamma/d_{\rm m}$ and/or values 336 for the mismatch scale $L_{\rm c}$ (investigated in Section 3.2.5). In Figure 2a each 337 curve represents a family of fractures with the same rock walls, but their 338 separation $(d_{\rm m})$ differs. The behavior of a parallel plate model corresponds to 339 the horizontal dashed line $d_{\rm h}/d_{\rm m} = 1$. For closure $\gamma/d_{\rm m} < 0.1$, the hydraulic 340

behaviour is close to the parallel plate model. For different fracture families, 341 fluid flow tends to be channelized and different hydraulic behaviors can be 342 observed for similar values of the fracture closure $\gamma/d_{\rm m}$. In agreement with 343 previous studies [e.g. Méheust and Schmittbuhl, 2001, 2003], we find that 344 the hydraulic behavior of rough fractures deviate monotonically from the 345 ideal parallel plate model as fracture closure is increased. Depending on the 346 geometry as determined by the random seed, the deviation from the parallel 347 plate model can be positive, which implies that the fracture is more conducive 348 to flow than a parallel plate with identical mean separation (flow-enhancing 349 behavior) [Méheust and Schmittbuhl, 2000]. If the deviation is negative, 350 then the fracture is characterized by flow-inhibiting behavior. Similar to 351 previous studies [Méheust and Schmittbuhl, 2001: Neuville et al., 2010b], we 352 see that, for most cases (75% of fracture families), the effective hydraulic 353 transmissivity at the scale of the fracture is reduced. 354

In order to better understand the origin of these differences in hydraulic 355 behaviour, we plot in Figures 2b-d some of the investigated aperture fields 356 $d_{\rm fr}(x,y)/d_{\rm m}$ for the highest closure considered, and in Figures 2e-g the cor-357 responding maps of local fluxes (2-D velocities) normalized by their mean 358 value $(\boldsymbol{q}/\|\boldsymbol{q}\|)$. In Figure 2b, we see a large channel oriented parallel to 359 the applied pressure gradient (from left to right), which constitutes a con-360 figuration favorable to flow as seen in Figure 2e. This fracture morphology 361 corresponds to the largest ratio $d_{\rm h}/d_{\rm m}$ in Figure 2a. Figure 2c shows the map 362 of the ratio $d_{\rm fr}(x,y)/d_{\rm m}$ for one of the fracture families considered in Figure 363 2a; this family demonstrates a moderate flow-inhibiting behavior (family A, 364 red markers). In this case, the fracture aperture field is characterized by 365 a main tortuous channel with smaller flow obstacles (Figure 2f). In Figure 366 2d a barrier is seen across the whole fracture that is perpendicular to the 367 applied pressure gradient. As shown in Figure 2g, this results in a strong 368 flow-inhibiting behaviour of the fracture (lowest ratio $d_{\rm h}/d_{\rm m}$ in Figure 2a). In 369 general, the resulting local fluxes in fractures vary over several orders of mag-370 nitude with a ratio of the local flux to the mean local flux, q/||q||, reaching 371 ~ 12 in some geometrical configurations. 372

Additional simulations with other mismatch scales, L_c , indicate, in agreement with Méheust and Schmittbuhl [2003], that the mismatch scale also has a critical impact on the flow channeling. We find that the mean hydraulic behavior of rough-walled fractures generally converges to the parallel plate estimate when the ratio L/L_c increases. These results are discussed later in relation to the resulting thermal behaviour (Section 3.2.5).



Figure 2: (a) Evolution of the ratio of the hydraulic aperture to the mechanical aperture, $d_{\rm h}/d_{\rm m}$, as a function of the fracture closure $\gamma/d_{\rm m}$ for 20 fracture families representing different fracture aperture topographies. The Hurst component is $\zeta = 0.8$ and the ratio of the fracture length to the correlation length is $L/L_{\rm c} = 1$. (b-d) Maps of $d_{\rm fr}(x,y)/d_{\rm m}$; for the fracture demonstrating the largest ratio $d_{\rm h}/d_{\rm m} = 1.56$ at the largest closure considered, $\gamma/d_{\rm m} = 0.56$ (b); for fracture family A (red markers in (a)), which exhibits a moderate flow-inhibiting behavior $d_{\rm h}/d_{\rm m} = 0.59$ at the largest closure considered, $\gamma/d_{\rm m} = 0.6$ (c); for the fracture demonstrating the smallest ratio $d_{\rm h}/d_{\rm m} = 0.18$ at the largest closure considered, $\gamma/d_{\rm m} = 0.56$ (d). (e-g) Maps of local fluxes (2-D velocities) normalized by the mean local flux from left to right, corresponding respectively to geometries (b-d).

379 3.2. Thermal behaviour

380 3.2.1. Thermal front definition

Figure 3 presents snapshots of the temperature field simulated using a 381 parallel plate fracture model and a rough fracture model. Here and through-382 out the paper (see Table 2), we consider as leading example the self-affine 383 fracture from family A shown on Figure 2c at closure $\gamma/d_{\rm m} = 0.46$. Fam-384 ily A is considered as a representative example since this fracture family 385 demonstrates moderate flow inhibiting behaviour as most natural rock frac-386 tures [Méheust and Schmittbuhl, 2001]. We calculate the non-dimensional 387 temperature anomaly as 388

$$\Delta T(x, y, z, t) = \frac{T(x, y, z, t) - T_{\text{rock}}}{T_{\text{inj}} - T_{\text{rock}}}.$$
(10)

The temperature distribution in the rough-walled fracture is highly het-389 erogeneous (Figure 3b) and the temperature evolution over time may differ 390 considerably even for points located close to each other (Figure 3e). Initially, 391 the thermal anomaly propagates along preferential large aperture channels 392 and reaches for instance points B, D and C of Figure 3b, whose temperature 393 evolution is shown in Figure 3e. At these points, the rate of change in tem-394 perature slows down after the first few tenths of seconds. A similar trend, 395 albeit less pronounced, is observed for a flat fracture (point A in Figure 3a). 396 On the contrary, the temperature at the points in regions of the fracture of 397 low local aperture has a slower dynamic (point E). Overall, the variation of 398 the temperature field over time and space is complex. As shown in Figure 3 399 (c) and (d), thermal plumes advance approximately 0.1 m into the rock ma-400 trix. These observations confirm that considering the thickness of the rock 401 matrix layer D = 2 m is sufficient to eliminate the boundary effect. 402

To evaluate how the temperature field is linked to the pressure gradient, 403 we use here the concept of a thermal front. The thermal front's velocity is 404 an essential parameter for a geothermal reservoir as the cold front arrival 405 associated with the (re-)injection of fluids causes a decrease of the temper-406 ature of the produced fluid, thus determining the longevity and economic 407 prospect of the system [e.g. Nottebohm et al., 2012]. Furthermore, a widely 408 used concept to characterize hydraulic properties from heat tracer tests is 409 based on measuring thermal velocities, that are generally derived from ther-410 mal breakthrough curves using predefined values between injection and initial 411 temperatures [Gossler et al., 2019]. We define the thermal front as the set of 412 locations at which $\Delta T = 1/2$ (black lines in Figure 3). 413

For both the parallel plate and heterogeneous fractures considered above, we find as expected that heat loss at the fracture walls creates a thermal front (black solid line in Figure 3) that is delayed relative to the fluid front (blue solid line in Figure 3) [e.g. Bodvarsson, 1972]. Thus, for the parallel plate fracture, when the fluid front is approaching the outlet of the fracture, the thermal front travels a normalized distance $x_{\rm PP}^*/L$ equal to 0.3 (Figure 3a).

In order to characterize how the thermal behavior evolves on average, we 421 consider the evolution of the thermal front with time. Figure 3b presents 422 an example of the thermal front advancement for the fracture family A, 423 $\gamma/d_{\rm m} = 0.46$ (black dashed lines). The front spreading pathway varies with 424 the local fluid velocity due to the roughness of the fracture aperture. As the 425 thermal front grows, heat fingers are developing along preferential flow paths 426 within the fracture plane, mainly in the middle region of the fracture. This 427 causes deviations of the thermal front position from its average x^*_{ROUGH}/L . In 428 the following, we characterize the advancement and the evolution of thermal 429 fronts in rough fractures and determine geometrical parameters of individual 430 fractures controlling this advancement. This is achieved by studying the 431 hydrothermal behavior of models with different fracture aperture patterns. 432 Furthermore, we compare the results with the reference case of a fracture 433 modeled with two parallel plates separated by a constant aperture $d_{\rm m}$ (i.e., 434 no self-affine spatial variations). The key geometric characteristic of the 435 studied fractures are presented in Table 2. 436



Figure 3: Comparison of temperature anomalies in a parallel plate fracture ((a) - fracture plane view and (c) - view of the mid-longitudinal cross section) and in a model with strong fracture roughness belonging to fracture family A (see Figure 2c), with $\gamma/d_m = 0.46$ and L/Lc = 1 ((b) - fracture plane view and (d) - mid-longitudinal cross-section view). The pressure gradient was chosen such that the Péclet number was the same for both simulations, Pe = 51. Both fractures have the same mechanical aperture. The fluid and thermal front profiles, shown by blue and black solid lines, respectively, are obtained at t = 900 s, that is slightly below the time $t_{\text{HS}h} = 920$ s necessary for a volume equal to the total volume of the fracture to flow through the fracture. Dashed black lines depict three thermal front profiles obtained at different times (t = 10, 100, 500 s). The letters A - E indicate the locations where the temperature evolution is observed in Figure (e). (e) Temperature as a function of time at location A for a parallel plate fracture (red line) and at locations B - E for the heterogenous fracture (black lines).

Test	Fracture family	Closure	Mechanical aperture	Correlation
ID				
		$\gamma/d_{ m m}$	$d_{\rm m},{ m mm}$	length $L/L_{\rm c}$
Test 1	family A	0.001 - 0.6	2.5×10^{-3} -1.5	1
Test 2	equivalent par-	—	2.5×10^{-3} -1.5	—
	allel plate			
Test 3	family A	0.05 - 0.6	1.25 - 15	1
Test 4	equivalent par-	—	1.25–15	_
	allel plate			
Test 5	family A	0.32 - 0.6	12.5-23	1
Test 6	equivalent par-	_	12.5-23	_
	allel plate			
Test 7	20 families	0.05 - 0.6	$1.25 \times 10^{-1} - 1.5$	1
Test 8	family A	0.02 - 0.6	5×10^{-2} -1.5	2, 4, 16

437 3.2.2. Influence of fracture closure

We now investigate how the roughness amplitude influences the thermal 438 behaviour of fractures from family A (Figure 2c), which exhibits a moderate 439 flow-inhibiting behavior (red markers in Figure 2a). To do so, we vary the 440 fracture closure $\gamma/d_{\rm m}$ by varying the fracture's mechanical aperture $d_{\rm m}$, while 441 keeping the same standard deviation for their height distributions, γ (Test 442 1, Table 2). Examples of fracture apertures generated on a 1024×1024 grid 443 are shown in Figure 4a. For small fracture closure $\gamma/d_{\rm m} = 0.02$ (Figure 4a 444 top), spatial variations of the aperture are negligible in comparison to the 445 mean aperture. As the fracture is closed, $\gamma/d_{\rm m} = 0.21, 0.40$ and 0.59 (Figure 446 4a from top to bottom), relative fluctuations of the aperture increase. 447

As a consequence of increased closure, flow channeling becomes more 448 important. This is shown in Figure 4b, where maps of local fluxes normalized 449 by the mean local flux are shown. In Figure 4b, for high closure cases, the 450 flow tends to avoid regions of small local apertures and, consequently, is 451 localized in a large aperture channel along the flow direction. This channel 452 can be seen across almost the whole fracture in Figure 4a (bottom maps). 453 The aperture of this channel is relatively small in the vicinity of the inlet and 454 in the vicinity of the outlet, leading to the flow-inhibiting behavior displayed 455 in Figure 2. Finally, Figure 4c presents the simulated temperature fields 456

 $_{457}$ (after 1000 s of injection) for different values of fracture closure.

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Figure 4: (a) Maps of the ratio $d_{\rm fr}(x, y)/d_{\rm m}$ for $\gamma/d_{\rm m} = 0.02, 0.21, 0.40$, and 0.59, for fracture family A. Blue colors indicate areas of small local aperture, while orange shadings denote larger apertures. (b) Maps of local fluxes (2-D velocities) normalized by the mean local flux. (c) Temperature anomaly induced after 1000 s of injection, which approximately corresponds to the time necessary to replace the total volume of the fracture. The thermal fronts are shown as black lines; the fluid flows from left to right and the hot fluid is injected from the left. The linear color scale is the same for all figures of each column.

As discussed above, one of the important characteristics of the geometry 458 of the mixing zone (where $0 < \Delta T < 1$) is the position and shape of the ther-459 mal front (black dashed lines in Figure 4). The shape of the thermal front 460 within the fracture is strongly correlated with the hydraulic flow. For small 461 values of fracture closure, the thermal front is almost straight and transverse 462 to the mean flow direction. However, the thermal front becomes less smooth 463 as $\gamma/d_{\rm m}$ increases, the pattern of temperature distribution becomes complex 464 with 'slow zones' forming in regions of low local fracture apertures and ther-465 mal fingers developing along preferential flow channels. Thus, for $\gamma/d_{\rm m}$ = 466 0.59, when the most advanced thermal finger passes half of the fracture's 467 length, the most delayed region of the thermal front are still in the vicinity 468 of the fracture inlet (Figure 4c bottom). Hence, the width of the thermal 469 front parallel to the flow direction increases as the fracture is closed. 470

In order to quantify the variability of thermal front velocities, we use the 471 results of Test 1 (Table 2) and observe how the mean position of the thermal 472 front x^*_{ROUGH} evolves with time. The standard deviation of the front position, 473 which quantifies its width along the mean flow direction, is plotted in Figure 474 5 against the position x^*_{ROUGH} , at positions y = [0, 0.01, 10] m. When the 475 roughness amplitude increases, the standard deviation of the front position 476 increases, implying that the thermal channeling effect is more pronounced, as 477 expected. We also note that the velocity of the thermal front decreases as the 478 fracture closure increases. The latter is related to the hydraulic behaviour 479 of the fracture, which tends to inhibit the hydraulic flow as shown in Figure 480 2a. 481



Figure 5: Mean position of the thermal front normalized by the fracture size, x_{ROUGH}^*/L , versus the standard deviation of the front position normalized by the fracture size, σ_{xROUGH}/L , for various fracture closure γ/d_{m} . Fracture family A, fracture closure $\gamma/d_{\text{m}}=0.001, 0.03, 0.10, 0.21, 0.32, 0.46, 0.60$ and L/Lc = 1. Blueish marker colors refer to open fractures, and magenta marker colors refer to more closed fractures.

We further verified this observation by comparing the results of hydrother-482 mal simulations in rough-walled fractures with simulations in parallel plate 483 fractures of identical mechanical aperture (Test 2, Table 2). Figure 6 presents 484 the evolution in time of the average velocity of the thermal front $v_{\rm ROUGH} =$ 485 x^*_{ROUGH}/t relative to the $v_{\text{PP}} = x^*_{\text{PP}}/t$, that is, the thermal front velocity in 486 a fracture modeled with a constant aperture $d_{\rm m}$. For a small fracture closure 487 $\gamma/d_{\rm m} = 0.05$, which corresponds to a nearly smooth aperture field, a parallel 488 plate model reproduces a similar thermal profile and the ratio $v_{\rm ROUGH}/v_{\rm PP}$ 489 is close to 1. As the fracture closure is increased, $\gamma/d_{\rm m} = 0.18, 0.32, 0.46$ 490

⁴⁹¹ and 0.60 (Figure 6), the velocity of thermal front becomes slower compared ⁴⁹² to thermal front velocity in parallel plate fractures with identical mechanical ⁴⁹³ aperture $v_{\text{ROUGH}} < v_{\text{PP}}$.



Figure 6: Time evolution of the average velocity of the thermal front normalized by the thermal front velocity in the equivalent parallel plate fracture (i.e, the parallel plate of aperture equal to the rough fracture's mechanical aperture $d_{\rm m}$), for fracture family A, fracture closures $\gamma/d_{\rm m} = 0.05, 0.18, 0.32, 0.46, 0.6, \text{ and } L/Lc = 1$. Square markers refer to fractures with large mechanical apertures $d_{\rm m}$, and circle markers refer to smaller apertures $d_{\rm m}$.

For all simulations, higher ratios of thermal front velocities $v_{\text{ROUGH}}/v_{\text{PP}}$ are observed close to the fracture inlet. Figure 6 also demonstrates that for small fracture closure $\gamma/d_{\text{m}} = 0.05$, $v_{\text{ROUGH}} > v_{\text{PP}}$, meaning that the thermal

front advances faster in rough fractures compared to what would be expected 497 with a parallel plate fracture of (uniform) aperture $d_{\rm m}$. However, after a 498 short transient regime, the thermal front velocities in rough and in smooth 499 fractures become equal, $v_{\rm ROUGH} = v_{\rm PP}$. As the thermal tracer enters the 500 fracture, heat diffuses first across the fracture, and, afterwards, away into the 501 matrix. Once the rock temperature starts to evolve in time and in space, the 502 ratio $v_{\rm ROUGH}/v_{\rm PP}$ stabilizes. Larger fracture apertures imply that heat needs 503 more time to diffuse across the fracture aperture. To verify this, we evaluate 504 through Tests 3-4 (Table 2) the thermal front velocity within the fractures in 505 family A with different mechanical apertures but the same fracture closures 506 $\gamma/d_{\rm m}$ (Figure 6). For a fracture with an aperture $d_{\rm m} = 15$ mm, the thermal 507 front velocity ratio becomes quasi-steady after t = 500 s, when the thermal 508 front has travelled a mean normalized distance x^*_{ROUGH}/L equal to 0.17. For 509 a fracture with the same closure, $\gamma/d_{\rm m} = 0.05$, but smaller aperture, $d_{\rm m} = 1.5$ 510 mm, the thermal front velocity ratio becomes quasi-steady after t = 200 s, 511 and for fractures with small apertures $d_{\rm m} < 1$ mm, the thermal front velocity 512 ratio stabilizes already after t = 100 s, when the thermal front has travelled a 513 mean normalized distance x^*_{ROUGH}/L of less than 0.1. We further evaluated 514 through Tests 5-6 (Table 2) that for more closed fractures (asterisk in Figure 515 6) with large apertures ($d_{\rm m} = 13 - 23$ mm), the thermal front velocity ratio 516 becomes quasi-steady after t = 400 - 700 s, respectively. 517

518 3.2.3. Influence of the fracture hydraulic aperture

For the same cases as in Figure 6, Figure 7 presents the ratio $v_{\rm ROUGH}/v_{\rm PP}$ 519 versus the ratio between the hydraulic and mechanical apertures $d_{\rm h}/d_{\rm m}$ for 520 two different times: for a very short duration t = 30 s, when the regime is 521 still transitory (grey markers), and for a longer duration, t > 700 s (black 522 markers), when the thermal front velocity ratio becomes quasi-steady. For a 523 short duration, we can observe that for a rough aperture, the thermal front 524 advances systematically faster in comparison to what we expect from the 525 hydraulic behavior (all the grey points are above the 1:1 line). Our results 526 also demonstrate that this effect is more pronounced for fractures with large 527 apertures (circle markers referring to small apertures are closer to the 1:1 528 line than square markers and asterisk referring to larger apertures). The 529 demonstrated faster propagation of the thermal signal in rough fractures 530 (v_{ROUGH}) when compared to that in smooth fractures (v_{PP}) agrees with the 531 work of Neuville et al. [2010b], who attributes this effect to a decrease in heat 532 exchange efficiency in rough fractures due to the reduction of transit times 533

⁵³⁴ in the channeled areas of a rough-walled fracture.

However, once the hosting rock temperature starts to evolve, a process 535 which was not accounted for in the model of Neuville et al. [2010b], the ther-536 mal front velocity in rough fractures slows down (Figure 6), and, for t > 400537 s, we obtain (Figure 7) a perfect correlation between the ratio $v_{\rm ROUGH}/v_{\rm PP}$ 538 and the ratio between the hydraulic and mechanical apertures $d_{\rm h}/d_{\rm m}$ (black 539 triangle markers). This implies that once heat has diffused along the out-540 of-plane direction over the fracture's aperture, the thermal behavior of a 541 rough-walled fracture is determined by its effective hydraulic transmissivity. 542 For the morphology investigated here (Family A fractures), the permeability 543 is reduced, and, thus, the advancement of the thermal front is slower in rough 544 fractures compared to what would be expected with a model of flat fractures 545 having the same mechanical aperture $d_{\rm m} (v_{\rm ROUGH}/v_{\rm PP} < 1)$. 546

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Figure 7: Ratio of the average velocity of the thermal front relative to that in the equivalent parallel plate model (same mechanical aperture) versus $d_{\rm h}/d_{\rm m}$, for fracture family A $(L/L_{\rm c}=1)$.

We now leave the specifics of family A and consider all fracture fami-547 lies in Figure 2a for different closure values (Test 7, Table 2). Statistical 548 thermal results presented in Figure 8 confirm the near-perfect correlation 549 between the ratio $v_{\rm ROUGH}/v_{\rm PP}$ and the ratio between the hydraulic and me-550 chanical apertures $d_{\rm h}/d_{\rm m}$. This means that, once stabilized, such that heat 551 has diffused along the out-of-plane direction over the fracture's aperture, the 552 mean position in time of the thermal front within a rough-walled fracture 553 is determined by the hydraulic aperture $d_{\rm h}$. For different fracture families 554 with the same fracture closure $\gamma/d_{\rm m}$, we find that the flow inhibiting be-555

havior is favored statistically [Méheust and Schmittbuhl, 2001]. Note that 556 these flow-enhancing or flow-inhibiting behaviors of individual fractures are 557 related to the fractures' hydraulic anisotropy, as a flow-enhancing fracture 558 becomes flow-inhibiting (and vice-versa) when the flow direction is rotated 559 by 90° (see discussion in Méheust and Schmittbuhl [2001]). Hence, as the 560 fracture, due to the roughness of its walls, is either less or more permeable 561 than a flat parallel plate of identical mechanical aperture, the efficiency in 562 transferring heat is also highly variable $(0.1 < v_{\rm ROUGH}/v_{\rm PP} < 1.6)$ from one 563 fracture family to another, but ratios smaller than 1 are favored statistically. 564

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Figure 8: Grey markers: averages of the normalized thermal front velocities $v_{\rm ROUGH}/v_{\rm PP}$ versus the ratio of hydraulic to mechanical apertures $d_{\rm h}/d_{\rm m}$, for more than 150 cases whose hydraulic apertures are presented in Figure 2 for various closure $\gamma/d_{\rm m}$ values, $\zeta = 0.8$, $L/L_{\rm c} = 1$. Red markers correspond to fracture family A and different mismatch scales $L/L_{\rm c} = 2, 4, 16$, respectively. The normalized thermal front velocities are considered at times larger than the time needed for heat to diffuse across the fracture aperture). Markers are transparent to highlight the density of points clustered near the 1 : 1 line, which holds for parallel plates separated by $d_{\rm h}$. The minimum root mean square error (RMSE) used to quantify the goodness-of-fit is 0.01.

565 3.2.4. Conductive heat flux

While previous studies characterized the heat exchange efficiency of rough fractures through the use of temperature metrics [Neuville et al., 2010a, 2013; Fox et al., 2015], in this study, we provide some insights into diffusive exchange processes at the fracture scale. Using the same data (Tests 1-2, Table

2), we now calculate the total conductive heat flux between the fracture 570 and the rock matrix for family A for different values of the fracture clo-571 sure, $\gamma/d_{\rm m} = 0.05, 0.18, 0.32, 0.46, 0.60$. Our results, presented in Figure 572 9, demonstrate that for all cases investigated here, the conductive heat flux 573 is greater for the equivalent parallel plate fracture (i.e., the parallel plate 574 with an aperture equal to the rough fracture's mechanical aperture $d_{\rm m}$): 575 $Q_{\rm ROUGH}^{(h)} < Q_{\rm PP}^{(h)}$. Moreover, the ratio $Q_{\rm ROUGH}^{(h)}/Q_{\rm PP}^{(h)}$ converges in time to a plateau (Figure 9, inset). Interestingly, Figure 9, showing the plateau value 576 577 versus the ratio of the hydraulic to mechanical apertures $d_{\rm h}/d_{\rm m}$, demon-578 strates that the conductive heat flux between the rough fracture and the 579 surrounding rock can be predicted from the equivalent parallel plate model. 580 Overall, for fracture family A, both the heat flux along the fracture and the 581 conductive heat fluxes between the fracture and the embedding rock decrease 582 when the roughness amplitude increases. This analysis suggests that a major 583 cause of the observed slowing down of the thermal front in rough fractures 584 compared to smooth fractures having the same mechanical aperture (Fig-585 ure 7) is related to the flow-inhibiting behavior of fractures from family A, 586 rather than to an increase in the efficiency of the conductive heat exchange 587 between the fluid and the rock matrix. Finally, this result confirms that for 588 the hydrothermal conditions studied here, when the influence of heat advec-589 tion in the fracture dominates the influence of conduction in the matrix, the 590 hydraulic aperture governs the fracture's thermal behaviour. As we shall dis-591 cuss in section 4, such conditions are actually relevant for most applications 592 (heat tracer testing and geothermal systems). 593



Figure 9: Steady state ratio of the total conductive heat flux between the fracture and the rock matrix to the same quantity measured in the equivalent parallel plate model (same mechanical aperture as the rough fracture) versus $d_{\rm h}/d_{\rm m}$, for fracture family A and $L/L_{\rm c}=1$. The RMSE is equal 0.005. The inset illustrates the evolution in time of that ratio before the thermal exchange quasi-steady state is reached.

⁵⁹⁴ 3.2.5. Influence of the mismatch scale/correlation length

Finally, we investigate how the mismatch scale (i.e., correlation length) influences the thermal behaviour of the fracture. To do so, we modify not only the fracture closure $\gamma/d_{\rm m}$, but also the ratio $L/L_{\rm c}$, while keeping the same numerical seed for the generation of the rough topographies, and the same standard deviation for their height distributions (Test 8, Table 2). Figure 10 presents the simulated temperature fields (after 1000 s of injection)

for different mismatch scales, $L/L_c = 2$ (Figure 10a), $L/L_c = 4$ (Figure 601 10b), $L/L_c = 16$ (Figure 10c), and for different values of fracture closure, 602 $\gamma/d_{\rm m} = 0.02, 0.25, 0.48,$ and 0.60 (from top to bottom). Similarly to 603 $L/L_{\rm c} = 1$ (Figure 4), the thermal channeling effect is all the more pro-604 nounced as the fracture is more closed (Figure 10). For $L/L_c = 2$ (Figure 605 10a), the thermal front displays large scale distortions representing a large 606 fraction of its total width. Furthermore, we observe the refinement of fila-607 ments and global flattening of thermal fronts (i.e., decrease in their roughness 608 amplitude) with increasing L/L_c (Figure 10 from left to right), which is de-609 termined by how the decrease of the mismatch scale impacts the advecting 610 velocity field, reducing the typical scale of its heterogeneities and the 2-D 611 velocity contrast between preferential flow paths and regions of lower veloc-612 ities. 613

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Increasing mismatch scales L/L_C —

Figure 10: Comparison of temperature anomalies induced after 1000 s of injection for different mismatch scales (a) $L/L_c = 2$, (b) $L/L_c = 4$ and (c) $L/L_c = 16$ and for different fracture closures: $\gamma/d_m = 0.02, 0.25, 0.48$, and 0.60.

Despite the changes in the q-field with increasing L/L_c , we find similarly 614 to what is observed for $L_c = L$ (black markers in Figure 8), that the fluid 615 flow scaling translates into that of heat transport. Indeed, red markers in 616 Figure 8 show strong correlation between the ratio $v_{\rm ROUGH}/v_{\rm PP}$ and the ratio 617 between the hydraulic and mechanical apertures $d_{\rm h}/d_{\rm m}$ for $L/L_{\rm c} = 2, 4,$ 618 and 16. This result confirms that the hydraulic behaviour allows predicting 619 thermal channeling effects and the related thermal behavior for geological 620 rough fractures for various values of the fracture closure and various values 621 of the ratio $L/L_{\rm c}$. 622

623 4. Discussion

We find that the thermal behavior of horizontal rough-walled fractures 624 can be predicted from their hydraulic behavior, as demonstrated for a wide 625 range of thermal Péclet numbers 6 < Pe < 200. Of course, this finding is 626 expected to be all the more valid for larger Péclet numbers (Pe > 200). For 627 lower Péclet values, slight deviations from this general finding was observed 628 for Pe = 5. Considering lower Péclet numbers would be very demanding in 629 terms of computational resources, but it would also not be so relevant for 630 applications. Indeed, Péclet numbers typically take values in the range of 631 10-7 000 in fractured geothermal systems under production [Horne and Ro-632 driguez, 1983; Geiger and Emmanuel, 2010; Neuville et al., 2010a], and the 633 Péclet numbers of the mal tracer tests range between 2 and 70 000 [Klepikova 634 et al., 2016; Hawkins et al., 2017; de La Bernardie et al., 2019], as summarized 635 in Table 3. This suggests a broad applicability of our inferred relationships 636 between heat transport and hydraulic behavior. Interestingly, similar conclu-637 sions have also been previously achieved for solute transport: applying the 638 equivalent aperture size calculated based on the equivalent permeability of 639 the system provides an acceptable prediction of solute transport [Nick et al., 640 2011 641

Study	Scale	Peclet number
Horne and Rodriguez [1983]	. Fracture network	10-100
Ge [1998]	Single fracture	5-100
Geiger and Emmanuel [2010]	Fracture network	14-145
Neuville et al. [2010a]	Single fracture	7 000
Neuville et al. [2013]	Single fracture	10
Klepikova et al. [2016]	Single fracture	5000
Hawkins et al. [2017]	Single fracture	2-8
de La Bernardie et al. [2019]	Single fracture	70 000

Table 3: Péclet numbers considered in previous studies on heat transport in fractured media.

In our model, fracture flow and heat transport are described in 2-D. This 642 allows us to solve transport both in the fracture and in the rock matrix, with 643 an extent of the matrix along the direction normal to the fracture plane that 644 is sufficiently large to avoid boundary effects. This wouldn't be possible if we 645 had to discretize the fracture aperture in a 3-D mesh within the fracture to 646 account for fracture flow and transport in 3-D, or it would be so demanding on 647 computer resources that we wouldn't be able to consider ensemble statistics of 648 fractures with identical geometrical parameters. Due to this choice, however, 649 3-D flow effects cannot be accounted for in our model. A number of studies 650 have addressed such effects, and concluded that they might be significant. 651 These include nonlinearities in the flow induced either by local tortuosity 652 and roughness, or by inertial effects [e.g Ge, 1997; Brush and Thomson, 653 2003; Wang et al., 2015, 2020; He et al., 2021]. The latter are not relevant 654 to our study, since we consider creeping flow. However, solving the flow 655 from the Reynolds equation (i.e. the traditional local cubic law), which 656 cannot account for tortuosity effects in the third dimension, can result in 657 overestimation of the transmissivity (or hydraulic aperture). Nevertheless, 658 in laminar flow regimes, contributions of these effects do not impact flow and 659 heat transport significantly [e.g. Brush and Thomson, 2003; Lee et al., 2015]. 660 The fracture's dimensionality may also impact heat transport through it. 661

We consider a horizontal fracture, and thus do not need to account for buoyancy effects (resulting from the temperature-dependence of the fluid's density), which, in a subvertical fracture, may lead to convective fluid circulation [Patterson et al., 2018]. Note that some studies solving advection-diffusion equations for heat transport in three dimensions report the emergence of

3-D effects. Thus, the presence of recirculation and stagnant zones related 667 to highly variable morphology of the fluid-rock interface may locally, within 668 the asperity, modify the heat exchange [Andrade et al., 2004; Neuville et al., 660 2013]. Another possible thermal effect was studied by Klepikova et al. [2016] 670 and de La Bernardie et al. [2019] and emerges when large local slopes (angle 671 between the orientation of the local fracture wall and that of the fracture 672 plane) exist, and the heat flux in between the matrix and the fracture, oc-673 curring dominantly in the direction perpendicular to the fracture walls, is 674 oriented locally at a large angle with respect to the fracture plane. This 675 effect was shown to have a significant impact on the scaling of heat recovery 676 in both space and time, and the findings were supported by field experiments 677 performed on the fractured rock site of Ploemeur, where high aperture chan-678 nels (around a few cm) participate to the transport of heat [Klepikova et al., 679 2016; de La Bernardie et al., 2019]. Still we do not expect that acounting 680 for 3-D effects of fracture geometry would have a significant impact on our 681 results. In contrast to Ploemeur field site, fractures walls in this study are 682 assumed to have small local slopes (this is essentially what the lubrication 683 approximation means). 684

The impact of the spatial resolution of the aperture roughness has also 685 been investigated. Additional simulations reported in the Appendix demon-686 strate that using slightly lower spatial resolution (i.e., downsampling the 687 aperture field by a factor up to 8) does not significantly modify the re-688 sults. These results are in general agreement with the studies of Méheust 689 and Schmittbuhl [2001] and Neuville et al. [2011]. The former demonstrated 690 that the Fourier modes of the aperture field corresponding to the largest 691 scales control flow channeling in the fracture plane for the most part, and 692 therefore, the fracture's hydraulic aperture, while the latter confirmed this 693 finding and further demonstrated that it also holds for heat transport in 694 rough fractures. 695

We do not consider the thermal stress acting on preferential flow paths, 696 which reduces the effective compressive stress along these paths and, thereby, 697 further exacerbates flow channeling, thus impacting heat exchange processes 698 [Guo et al., 2016; Salimzadeh et al., 2018; Patterson and Driesner, 2020]. As 699 demonstrated by recent works of Guo et al. [2016]; Patterson and Driesner 700 [2020], the magnitude of the changes due to thermo-mechanical effects is 701 comparable with the magnitude of the initial aperture variation. We have 702 chosen to ignore such thermal-hydraulic-mechanical-chemical (THMC) cou-703 plings for two reasons. First, we sought to quantify the impact of fracture 704

surface roughness on heat transport and exchange with the rock matrix, and 705 wanted to discriminate these purely geometrical effects from those related 706 to thermo-mechanical couplings. Second, since THMC processes (i) arise in 707 Enhanced/Engineered Geothermal Systems (EGS) when strong contrasts in 708 temperature exist and (ii) are relatively slow (effects on reservoir performance 709 are noticeable over a time scale of months-years) [Pandey et al., 2014; Guo 710 et al., 2016; Salimzadeh et al., 2018]. Consequently, such effects are expected 711 to be negligible within the typical duration of heat tracer tests, which is our 712 prime target application. Introducing THMC couplings in the model is ex-713 pected to produce stronger channeling and consequently a larger deviation of 714 the fracture's hydraulic behavior from that of the smooth fracture (parallel 715 plate) of aperture equal to the rough fracture's mean aperture. Since this 716 would result in a change in fracture surface topography, we would still expect 717 the main finding of the present study to hold, namely, that heat transport 718 behavior can be predicted from the hydraulic behavior of the fracture. 719

720 5. Conclusions

We have investigated numerically the influence of the statistical proper-721 ties of the aperture field and upscaled hydraulic behavior on heat transport in 722 rough rock fractures with realistic geometries. The flow regime was assumed 723 to be laminar and at low Reynolds number, and the gradient of the aper-724 ture field to be small (lubrication approximation), so that flow in the frac-725 ture could be modeled by the Reynolds equation in the 2-D fracture plane. 726 We considered a regime where heat transport in the fracture is moderately 727 dominant with respect to heat conduction in the rock matrix (Pe = 51), 728 a configuration which is relevant for practical situations at geothermal sites 729 and for forced hydraulic conditions usually adopted during field heat tracer 730 tests. We analyzed 20 rough topographies with a Hurst exponent $\zeta = 0.8$, 731 with aperture closures $\gamma/d_{\rm m}$ varying from 0.001 to 0.6 over a wide range of 732 mean fracture apertures, and with four different values of the mismatch scale 733 $L/L_{\rm c} = 1, 2, 4, 16.$ 734

At fixed fracture closure, the deviation from the parallel plate model increases as L_c is decreased. When closing the fracture, the deviation of the hydraulic and thermal behaviors from the equivalent parallel plate model increases. In general, the thermal behaviour is highly variable among a population of fractures with identical geometrical parameters. In comparison to a fracture of uniform aperture equal to the rough fracture's mechanical ⁷⁴¹ aperture, 75% of the considered fracture aperture fields exhibit a slower dis⁷⁴² placement of the thermal front along the fracture and less thermal exchange
⁷⁴³ between the fracture and the surrounding rock.

Our main finding is that under the considered conditions, thermal be-744 haviour of rough-walled rock fractures only depends on the hydraulic prop-745 erties. A similar conclusion was reached by Neuville et al. [2010b], who found 746 that the hydraulic aperture is a better parameter than closure to assess the 747 thermal exchange efficiency of rough fractures. In stark contrast to Neuville 748 et al. [2010b], we found that the heat transport along rough-walled fractures 740 was similarly efficient as a parallel plate (i.e., smooth) fracture of identical 750 hydraulic transmissivity. The thermal fronts in rough fractures are initially 751 slightly more advanced (at identical times) than thermal fronts in flat frac-752 tures with equivalent permeabilities, but this holds only for a very short time 753 (i.e., the time needed for heat to diffuse along the out-of-plane direction over 754 the fracture's aperture). Depending on the mean fracture aperture, this tran-755 sition period lasts for tens to a few hundreds of seconds, during which the 756 thermal front travels a mean normalized distance x^*_{ROUGH}/L equal to ~ 0.1. 757 By accounting for fracture-matrix heat exchange by transverse diffusion, a 758 process which was neglected by Neuville et al. [2010b], the thermal behavior 759 of a rough-walled fracture is found to be controlled by its hydraulic aper-760 ture and boundary conditions. This striking novel finding results from an 761 improved description of the coupled flow and heat transport. 762

The practical implication of our finding is that thermal exchanges at the 763 scale of a single fracture is controlled by the effective hydraulic transmissiv-764 ity. Provided that thermal properties of the host rock are known, this implies 765 that (1) heat tracer tests are reliable for inferring effective fracture transmis-766 sivity, and (2) the geothermal efficiency can be computed at field sites using 767 hydraulic characterization alone. Furthermore, as long as the considered 768 time scale doesn't allow for significant THM(C) coupling to take place, it 769 follows that the temporal evolution of the geothermal efficiency can be pre-770 dicted over significantly large time scales using well-known low-dimensional 771 hydraulic parameterizations in terms of effective hydraulic properties. 772

Future work could address non-Stokes flow conditions (i.e., laminar but non-linear flow) in the fracture. Another interesting prospect is the overall large-scale heat transport behavior in a fractured geological formation. It is expected to depend on the combined effects of both the local scale heterogeneity of individual fractures and the heterogeneity at the scale of a discrete fracture network (DFN) consisting of multiple intersecting fractures.

The study of coupled flow and heat transport in such DFNs will be the topicof future work.

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Appendix: Impacts of the spatial resolution on the hydraulic and thermal results

We use the same finite-difference numerical scheme as described previ-783 ously to compute the flow and temperature fields in downsampled apertures, 784 that is, the aperture field $d_{\rm fr}(x,y)$ is only considered at every *n*-th point of 785 the grid, where n = 2, 4, 8. In Figure 11a, the relative difference between hy-786 draulic aperture d_h for the downsampled apertures and the hydraulic aperture 787 with full resolution of the geometric aperture, $d_{h,ref}$, is evaluated. All com-788 puted hydraulic apertures are closer than 0.4 per cent to the full resolution 789 $d_{h,\text{ref}}$. In general, our results reveal that d_h is overestimated with respect to 790 $d_{h,\text{ref}}$ when decreasing the spatial resolution. The relative difference between 791 the average velocity of the thermal front calculated inside the downsampled 792 apertures and apertures with full resolution is shown on Figure 11b for the 793 case of the largest closure considered, $\gamma/d_{\rm m} = 0.6$. Here, the precision of the 794 approximation is better than 0.6 per cent. 795



Figure 11: (a) Relative errors of predicted hydraulic apertures d_h when downsampling the aperture data by a ratio 2, 4, and 8; the errors are plotted as a function of the fracture closure. Fracture family A (see Figure 2c), L/Lc = 1. (b) Relative errors made on the average velocity of the thermal front v_{ROUGH} , plotted as a function of the downsampling ratio. Fracture family A, with $\gamma/d_m = 0.6$ and L/Lc = 1.

796 Notation

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Symbol list	
C_{p}	heat capacity
$d_{\mathrm{fr}}(x,y)$	fracture aperture field
$d_{ m m}$	mechanical aperture
$d_{ m h}$	hydraulic aperture
D	thickness of the rock matrix
k	thermal conductivity
L	fracture length
$L_{\mathbf{c}}$	mismatch scale (correlation length)
P	local pressure
Pe	Péclet number ($Pe = u_{\rm M} d_{\rm m} \rho_{\rm f} C_{\rm p,f} / k_{\rm r}$)
q	local flux or 2D velocity, i.e.,
	the integral over the local fracture aperture of \boldsymbol{u}
Q	flux through the fracture
$Q^{(h)}$	conductive heat flux between fracture and rock matrix,
	over the the entire fracture walls' areas
Re	Reynolds number $(Re = d_{\rm m} u_{\rm M}/\eta)$
t	time
T(x, y, z, t)	temperature
$\Delta T(x, y, z, t)$	non-dimensional temperature anomaly,
	$\Delta T(x, y, z, t) = T(x, y, z, t) - T_{\text{rock}} / (T_{\text{inj}} - T_{\text{rock}})$
$T_{ m inj}$	injection temperature
$T_{ m rock}$	initial temperature
\boldsymbol{u}	three-dimensional fluid velocity in the fracture
$u_{ m M}$	maximum velocity within a parallel flat wall fracture
v	average velocity of the thermal front
x	distance along applied pressure gradient
x^*	mean position of the thermal front
y	distance normal to applied pressure gradient
z	out of fracture plane distance
γ	standard deviation of the aperture field
η	dynamic viscosity
ho	density
ζ	the Hurst (or, roughness) exponent

798

799	Subscripts	
	f	fluid
	${ m fr}$	fracture
800	r	rock
	ROUGH	rough fracture
	PP	parallel plate fracture

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Declaration of interests

 \boxtimes The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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