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1 **Three-dimensional natural convection, mixing and entropy**
2 **generation in heterogeneous porous medium**

3

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4 **Abstract**

5 Three-dimensional (3D) natural convection (NC) processes in heterogeneous porous media
6 and associated energy losses and mixing processes are still poorly understood. Studies are
7 limited to two-dimensional domains because of computational burden, worsened by
8 heterogeneity, which may demand grid refinement at high permeability zones for accurate
9 evaluation of buoyancy forces. We develop a meshless Fourier series (FS) solution of the
10 natural convection problem in a porous enclosure driven by thermal or compositional
11 variations. We derive the vector potential formulation of the governing equations for vertical
12 and horizontal heterogeneity of hydraulic conductivity and implement an efficient method to
13 solve the spectral system with an optimized number of Fourier modes. 3D effects are induced
14 either by heterogeneity or variable boundary conditions. The developed FS solution is verified
15 against a finite element solution obtained using COMSOL Multiphysics. We evaluate entropy
16 generation (viscous dissipation and mixing) indicators using Fourier series expansions and
17 assess how they are affected by heterogeneity. We define a large-scale Rayleigh number to
18 account for heterogeneity by adopting an arithmetic average effective permeability. Results
19 show that increasing the Rayleigh number intensifies fluid flow, thus enhancing convective
20 transfer, which causes a dramatic increase in total entropy generation. Both viscous
21 dissipation and mixing (and thus chemical reactions in the solute transport case) increase. The
22 third dimension effect, which also enhances flow and entropy indicators, is more pronounced
23 at high Rayleigh numbers. Surprisingly, entropy variation indicators remain virtually
24 unchanged in response to changes in heterogeneity, for fixed Rayleigh number, which we
25 attribute to the arithmetic average permeability being indeed appropriate for NC in 3D. This
26 study not only explores the effect of Rayleigh number and heterogeneity on natural
27 convection processes and the associated entropy generation and mixing processes, but also
28 provides a highly accurate solution that can be used for codes benchmarking.

29

30 **Keywords:** Natural convection; Entropy generation; Heterogeneous porous media; Three-
31 dimensional; Fourier series method

32 **1 Introduction**

33 Natural convection (NC) takes place in porous media when the saturating fluid density
34 changes due to the variation of temperature and/or composition. Because of its wide
35 applications in environmental, industrial, and engineering fields, NC in porous enclosures
36 caused by thermal effects has been intensively investigated in the past decades. These
37 applications range from the small (micrometers) scale, such as blood flow in the pulmonary
38 alveolar sheet and heating process in solid oxide fuel cells, to the large (meters or kilometers)
39 scale, such as thermal insulation in buildings, CO₂ sequestration, aquifers thermal energy
40 storage, seawater intrusion and geothermal or oil reservoirs. Comprehensive surveys on NC in
41 porous media and its industrial and environmental applications can be found in [Nield and](#)
42 [Simmons \[2019\]](#), [Nield and Bejan \[2017\]](#), [Vafai \[2011\]](#), [Vadász \[2008\]](#), [Ingham and Pop](#)
43 [\[2005\]](#) and [Kimura et al. \[1997\]](#).

44 Energy losses due to the convective heat transfer, fluid friction, and diffusion effects occur in
45 practical applications involving heat transfer in porous media [[Torabi et al., 2017](#)]. This
46 energy loss or the process efficiency can be quantified in terms of entropy generation, based
47 on simultaneous application of the first and second laws of thermodynamics. Entropy
48 generation analysis is usually applied to distinguish between reversible and irreversible
49 processes. By evaluating and minimizing the entropy generation, the overall efficiency of a
50 thermal system can be improved, and losses can be optimized. Special attention has been paid
51 to the study of entropy generation on NC in porous enclosures. The main addressed topics are
52 the influence on entropy generation of enclosure's geometry and boundary conditions [[Baytaş,](#)
53 [2000](#); [Kaluri and Basak, 2011](#); [Basak et al., 2012^{a,b}](#); [Datta et al., 2016](#); [Chamkha and](#)
54 [Selimefendigil, 2018](#); [Chandra Pal, 2018](#)], hydraulic and thermal parameters of the porous
55 medium [[Bouabid et al. 2011](#); [Chamkha and Selimefendigil, 2018](#)], different types of fluids
56 under different rheological behaviors [[Khan and Gorla, 2011](#); [Al-Zamily, 2017](#); [Mansour et](#)

57 [al., 2017](#)] or internal heat generation [[Al-Zamily, 2017](#)]. [Mansour et al. \[2017\]](#) investigated
58 the effect of viscous dissipation. [Jbara et al. \[2013\]](#) studied entropy generation under unsteady
59 conditions. While most studies assume thermal equilibrium between solid and liquid phases of
60 the porous medium, [Baytas \[2007\]](#) addressed entropy generation under non-equilibrium
61 thermal conditions. Entropy generation in MHD nanofluid natural convection has been
62 investigated in [Ghasemi and Siavashi \[2017\]](#). [Oztop and Al-Salem \[2012\]](#) presented a
63 thorough review of entropy generation in natural and mixed convection. Several studies are
64 concerned with the effect of coupled mass and heat transfer processes (i.e., double-diffusive
65 convection) on entropy generation [[Mchirgui et al. 2014](#); [Kefayati, 2016](#); [Hussain et al., 2018](#)].

66 Two different kinds of processes drive entropy generation on NC problems: dissipation of
67 mechanical energy by viscous forces and loss of variability by diffusion (conduction in
68 thermal convection, or molecular diffusion in solute transport). The latter has received
69 increased attention in the reactive transport literature, where it is termed mixing, because it
70 drives chemical reactions [[Rezaei et al., 2005](#); [Cirpka and Valocchi, 2007](#)]. In fact, the rates
71 of fast reactions, driven by the rate at which reacting solutes mix, are proportional to the local
72 entropy generation rate [[de Simoni et al., 2005](#)].

73 Heterogeneity of porous media is known to play a significant role in flow and heat transfer
74 processes. Industrial and natural porous media display spatial variability of thermal and,
75 especially, hydraulic properties, such as permeability and thermal conductivity, which
76 significantly affect water flow and heat transfer. The effect of heterogeneity on NC in porous
77 media has been heavily scrutinized. A widely-discussed topic is the effect of heterogeneity on
78 the onset of NC induced by a vertical density gradient (unstable configuration) [[Nield and
79 Simmons, 2007](#); [Nield and Kuznetsov, 2007^{a,b}, 2008, 2011](#); [Nield, 2008](#); [Nield et al. 2009,
80 2016](#); [Simmons et al., 2010](#)]. The topic is especially relevant for geological CO₂ storage,
81 where density changes when CO₂ is dissolved in native fluids, because dissolution controls

82 the ultimate fate of CO₂, so that the onset of NC controls whether dissolution is going to be
83 relevant during CO₂ injection [Riaz et al., 2006; Hidalgo et al., 2009, 2012]. Impacts of
84 heterogeneity on the onset of NC under local non-equilibrium conditions have been studied in
85 Nield and Kuznetsov [2015]. Nguyen et al. [2016] studied the effects of heterogeneity on
86 fingering phenomena induced by unstable NC. The influence of heterogeneity on stable
87 configuration of NC (horizontal density gradient) has been the subject of several studies.
88 Marvel and Lai [2010] investigated NC in layered porous cavity. Fahs et al. [2015] studied the
89 effect of stratified heterogeneity on stable natural convection and provided a reference
90 solution for code benchmarking. Fajraoui et al. [2017] performed a global sensitivity analysis
91 to evaluate the effects of uncertainties related to parameters controlling the heterogeneity on
92 convective flow, temperature field, and heat transfer flux.

93 Most of above-mentioned studies on NC in porous enclosures and related processes'
94 irreversibility are limited to two-dimensional (2D) domains. This 2D assumption is commonly
95 adopted to reduce the computational overheads of three-dimensional (3D) simulations.
96 However, NC processes are three-dimensional by nature. The 2D assumption is only
97 applicable for configurations with specific geometry, boundary conditions, and heterogeneity,
98 where the variations are negligible in the third dimension. With the advancement of
99 computational technology, several 3D numerical studies have been conducted to investigate
100 and understand the three-dimensional NC processes. Pau et al. [2010] demonstrated that the
101 onset time is shorter and the convection rate is larger for 3D simulations than for 2D. Wang et
102 al. [2010] investigated 3D NC in an inclined porous cubic box under time oscillating
103 boundary conditions, where the 3D effect is related to box inclination. They found that the
104 convective flow was quasi-two-dimensional if the box has a moderate inclination angle, while
105 for seriously inclined cases, much more complicated three-dimensional convective flow
106 patterns were observed. Voss et al. [2010] investigated an unstable configuration of NC in an

107 inclined cubic box and showed the effect of 3D processes on the critical Rayleigh number for
108 the onset of instability. [Guerrero-Martínez et al. \[2016\]](#) studied unstable configuration
109 (vertical density gradient) of an inclined cubic box in both homogeneous and layered porous
110 domains, respectively.

111 This informal survey indicates evidence of the importance of heterogeneity in controlling NC
112 processes and the significance of entropy generation associated with NC in porous enclosures.
113 It also reveals increasing interest in 3D studies for practical purposes. However, this review
114 also shows that there are still several open research questions related to this topic. Indeed, due
115 to high computational requirements, 3D studies on NC in porous enclosures are scarce. While
116 different properties of domain and boundary conditions could lead to three-dimensional
117 configurations, in the few existing studies, the 3D effects are only induced by box inclination
118 or unstable flow configurations. Furthermore, to deal with computational overheads, existing
119 studies have considered relatively low Rayleigh numbers. In addition, 3D studies on NC
120 processes and associated entropy generation in heterogeneous domains are missing and
121 corresponding processes are still not well-understood. To the best of our knowledge, the only
122 existing work addressing this topic is [Zhuang and Zhu \[2018\]](#). Nevertheless, that work does
123 not account for real 3D effects as the problem under investigation can be simplified to 2D.
124 The main goal of this work is to address these gaps and to provide a new insight on NC and
125 entropy generation in 3D heterogeneous porous enclosures.

126 Thus, we study NC and entropy generation in a cubic enclosure filled with a heterogeneous
127 porous medium. This is a problem that has been widely studied in academic research and
128 engineering applications to understand NC processes [[Zhao et al., 2005, 2009](#)]. It is also a
129 typical problem that is commonly used as a benchmark to validate numerical codes. We
130 consider two different configurations corresponding to vertical and horizontal heterogeneity,
131 which are common in geological formations [[Jiang et al., 2010](#); [Miroshnichenko et al., 2018](#);

132 [Fahs et al., 2015](#)]. Both configurations are effective 3D cases that cannot be simplified to 2D.
133 The 3D effects are induced either by the heterogeneity of the porous domain or boundary
134 conditions. Simulation of three-dimensional NC in porous media is a computationally
135 challenging problem, particularly for high Rayleigh numbers. Heterogeneity compounds these
136 challenges as it leads to locally high permeability zones where the accurate evaluation of
137 buoyancy forces requires unpractical dense computational grids. Accurate evaluation of
138 entropy generation is also a hard computational task because it involves fluxes and space
139 derivatives of the temperature, which requires appropriate numerical techniques [[Younes et al.,](#)
140 [2010](#)]. Thus, to avoid computational limitations and numerical artifacts of conventional
141 methods, we develop an efficient and accurate meshless solution based on the Fourier series
142 method (FS) applied to the vector potential formulation of the governing equation [[Peyret,](#)
143 [2002](#); [Shao et al., 2018](#)]. We extend the vector potential formulation developed by [Shao et al.](#)
144 [[2018](#)] to the heterogeneous domain and we use an efficient technique to reduce the number
145 of Fourier series modes. Contrarily to the homogeneous domain, heterogeneity leads to full
146 non-zero vector potential. We use appropriate techniques to efficiently solve the spectral
147 system. This includes a simplified evaluation of the nonlinear convective terms, the use of an
148 efficient nonlinear solver, and parallel implementation of the FS method. Entropy generation
149 is evaluated analytically based on the Fourier series expansion. The developed FS solution is
150 verified by comparison against COMSOL Multiphysics. Taking advantage of the accuracy of
151 the FS solution, we provide high-quality data that can be used as a reference for the validation
152 of numerical codes dealing with NC and entropy generation. This represents an important
153 feature of this work, as reference benchmark solutions for entropy generation are lacking. Due
154 to its high performance, the FS solution is used to i) develop a parametric study, ii) to
155 understand the effect of heterogeneity on metrics characterizing temperature, heat flux,

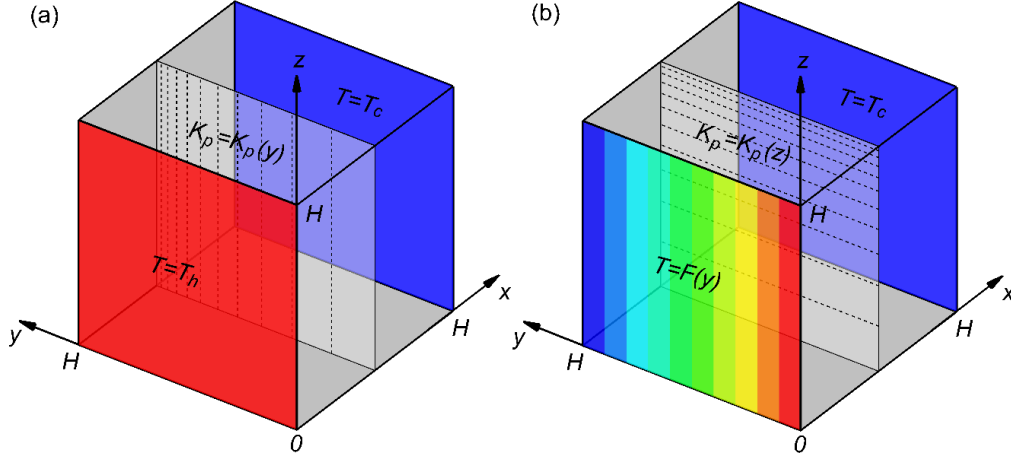
156 convective flow, mixing, and entropy generation, and iii) to evaluate the significance of the
157 3D processes by comparing 3D and 2D simulations.

158 **2 Problems description and governing equations**

159 We consider a cubic saturated porous enclosure of size H , as shown in Fig. 1, where fluid
160 flows in response to density variations caused by variations in temperature or concentration.
161 For simplicity, we adopt heat transfer nomenclature, but the problem is mathematically
162 equivalent to solute mass transfer. All domain boundaries are assumed impermeable, that is,
163 convective fluxes across the six sides are zero. Two different configurations of heterogeneity
164 are investigated in this work (Fig. 1). In the first configuration (V-het), the enclosure is filled
165 with vertically stratified porous media, so that its permeability varies along the y coordinate
166 (i.e., $k_p = k_p(y)$). The enclosure is subject to constant but distinct temperatures on two opposite
167 boundaries, i.e., $T = T_h$ at $x = 0$ and $T = T_c$ at $x = H$, as shown in Fig. 1(a). In the second
168 configuration (H-het), the enclosure is filled with horizontally stratified porous media, so that
169 its permeability is a function of z . This configuration can be simplified to 2D. But, as our
170 objective is to investigate effective 3D cases, we assume varying boundary temperature on
171 one side (i.e., $T = F(y)$ at $x = 0$), and constant temperature on the opposite side (i.e., $T = T_c$ at
172 $x = H$), as shown in Fig. 1(b). Variable temperature boundary conditions are common in the
173 simulations of geothermal reservoirs. The two configurations allow us to investigate the 3D
174 effects induced either by heterogeneity or from the varying temperature boundary conditions.

175

176



177

178 **Fig. 1.** Schematic description of the two cubic porous enclosures and their boundary
 179 conditions: (a) an enclosure filled by vertically stratified porous media with constant but
 180 distinct temperatures on the opposite boundaries (V-het); (b) an enclosure filled by
 181 horizontally stratified porous media with varying temperature on one side, and constant
 182 temperature on the opposite side (H-het).

183

184 The mathematical model describing the NC processes in saturated porous media is based on
 185 the mass conservation equation, Darcy's law, and the heat transfer equation. Adopting the
 186 Boussinesq approximation and steady-state fluid flow, these equations can be written as:

187

$$\nabla \cdot \mathbf{q} = 0 \quad (0)$$

188

$$\mathbf{q} = -\frac{k_p}{\mu} (\nabla p - \rho_c g \beta (T - T_c) \mathbf{e}_z) \quad (0)$$

189

$$C_m \frac{\partial T}{\partial t} + C_f \mathbf{q} \cdot \nabla T = \lambda_m \nabla \cdot \nabla T \quad (0)$$

190

where \mathbf{q} [LT^{-1}] is water flux (Darcy velocity), μ [$\text{ML}^{-1}\text{T}^{-1}$] is the dynamic viscosity of the

191

fluid, p [$\text{ML}^{-1}\text{T}^{-2}$] is pressure, ρ_c [ML^{-3}] is the density of fluid at the reference

192

temperature T_c , g [LT^{-2}] is the gravity acceleration, β [Θ^{-1}] is the thermal expansion

193

coefficient, k_p [L^2] is the permeability, which depends on the properties of the porous media

194

and may vary in space, t [T] is time, C_f [$\text{L}^{-1}\text{MT}^{-2}\Theta^{-1}$] is the thermal capacity (specific heat

195

times density) of the fluid, C_m [$\text{L}^{-1}\text{MT}^{-2}\Theta^{-1}$] and λ_m [$\text{MLT}^{-3}\Theta^{-1}$] are the thermal capacity

196 (specific heat times density) and the effective thermal conductivity of the porous medium,
 197 respectively. The latter is obtained by averaging the thermal capacity and conductivity of the
 198 fluid and solid phases, weighted by the porosity ε :

$$199 \quad C_m = \varepsilon C_f + (1 - \varepsilon) C_s \quad (0)$$

$$200 \quad \lambda_m = \varepsilon \lambda_f + (1 - \varepsilon) \lambda_s \quad (0)$$

201 Subscripts m, s, and f represent the porous medium, solid, and fluid, respectively. The density
 202 of the fluid is a linear function of temperature:

$$203 \quad \rho = \rho_c (1 - \beta(T - T_c)) \quad (0)$$

204 The boundary conditions of the two aforementioned configurations (V-het and H-het) are
 205 defined in Table 1, where q_x , q_y , and q_z are the water flux components in the x -, y -, and z -
 206 directions, respectively.

207 **Table 1.** Boundary conditions of the two configurations showing the variable prescribed
 208 temperature at the $x=0$ face.

Configuration	$x = 0$	$x = H$	$y = 0, H$	$z = 0, H$
V-het	$q_x = 0, T = T_h$	$q_x = 0, T = T_c$	$q_y = 0, \frac{\partial T}{\partial y} = 0$	$q_z = 0, \frac{\partial T}{\partial z} = 0$
H-het	$q_x = 0, T = F(y)$			

209

210 **3 Fourier series solution**

211 The Fourier series method is used to solve the governing equations for both configurations V-
 212 het (vertical heterogeneity) and H-het (horizontal heterogeneity). The solution procedure is as
 213 follows. First, governing equations are expressed in terms the vector potential. Second, a
 214 change of variables is made to ensure periodic-homogeneous boundary conditions for both
 215 flow and heat transfer. Third, the temperature and the components of the vector potential are
 216 expanded using Fourier series truncated at given orders, which are then substituted into the
 217 governing equations. After the Galerkin treatment, a system of nonlinear equations with the

218 Fourier series coefficients as unknowns is generated. Eventually, solving the system of
 219 equations, one obtains the vector potential and the temperature field expressed analytically in
 220 terms of Fourier coefficients.

221 3.1 The vector potential formulation

222 At steady state, Darcy's velocity \mathbf{q} admits a vector potential $\boldsymbol{\phi}$ such that $\mathbf{q} = \nabla \times \boldsymbol{\phi}$.
 223 According to the continuity equation, the vector potential satisfies $\nabla \cdot \mathbf{q} = \nabla \cdot (\nabla \times \boldsymbol{\phi}) = 0$.
 224 Applying the *curl* operator on Darcy's law, one can eliminate the fluid pressure in the flow
 225 equation as $\nabla \times \nabla p = 0$. Further, considering a solenoidal vector potential as shown in
 226 Guerrero-Martínez et al. [2016] and Shao et al. [2018] leads to $\nabla \cdot \boldsymbol{\phi} = 0$. Then assuming the
 227 permeability satisfies the function $K_p = K_p(y, z)$ due to the heterogeneity of the porous
 228 medium, one obtains the steady-state flow equations in terms of vector potential components:

$$229 \begin{cases} \nabla^2 \phi_x + \frac{1}{k_p} \left(\frac{\partial k_p}{\partial y} \left(\frac{\partial \phi_y}{\partial x} - \frac{\partial \phi_x}{\partial y} \right) - \frac{\partial k_p}{\partial z} \left(\frac{\partial \phi_x}{\partial z} - \frac{\partial \phi_z}{\partial x} \right) \right) + \frac{\rho_c g k_p \beta}{\mu} \frac{\partial T}{\partial y} = 0 \\ \nabla^2 \phi_y + \frac{1}{k_p} \frac{\partial k_p}{\partial z} \left(\frac{\partial \phi_z}{\partial y} - \frac{\partial \phi_y}{\partial z} \right) - \frac{\rho_c g k_p \beta}{\mu} \frac{\partial T}{\partial x} = 0 \\ \nabla^2 \phi_z - \frac{1}{k_p} \frac{\partial k_p}{\partial y} \left(\frac{\partial \phi_z}{\partial y} - \frac{\partial \phi_y}{\partial z} \right) = 0 \end{cases} \quad (0)$$

230 Substituting the vector potential into Eq. (3), we simplify the steady-state heat transfer
 231 equation to:

$$232 (\nabla \times \boldsymbol{\phi}) \cdot \nabla T = \alpha \nabla \cdot \nabla T \quad (0)$$

233 where $\alpha = \lambda_m / C_f$ represents the effective thermal diffusivity. Then we define the following
 234 dimensionless variables:

$$235 \Psi = \frac{\boldsymbol{\phi}}{\alpha}, \mathcal{G} = \frac{T - T_c}{\Delta T}, X = \frac{x}{H}, Y = \frac{y}{H}, Z = \frac{z}{H} \quad (0)$$

236 where $\Delta T = T_h - T_c$ is the temperature difference between the hot and cold walls. Using the
 237 above non-dimensional variables, we obtain the dimensionless steady-state flow and heat
 238 transfer equations as follows:

$$\begin{cases}
 \nabla^2 \psi_x + \frac{1}{k_p} \left(\frac{\partial k_p}{\partial Y} \left(\frac{\partial \psi_Y}{\partial X} - \frac{\partial \psi_X}{\partial Y} \right) - \frac{\partial k_p}{\partial Z} \left(\frac{\partial \psi_X}{\partial Z} - \frac{\partial \psi_Z}{\partial X} \right) \right) + Ra \frac{\partial \mathcal{G}}{\partial Y} = 0 \\
 \nabla^2 \psi_Y + \frac{1}{k_p} \frac{\partial k_p}{\partial Z} \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) - Ra \frac{\partial \mathcal{G}}{\partial X} = 0 \\
 \nabla^2 \psi_Z - \frac{1}{k_p} \frac{\partial k_p}{\partial Y} \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) = 0
 \end{cases} \quad (0)$$

$$(\nabla \times \boldsymbol{\psi}) \cdot \nabla \mathcal{G} = \nabla \cdot \nabla \mathcal{G} \quad (0)$$

241 where $Ra = \rho_c g k_p H \beta \Delta T / (\mu \alpha)$ is the local thermal Rayleigh number that is dependent on the
 242 variation of permeability in heterogeneous porous media.

243 These equations are similar to those of [Shao et al. \[2018\]](#), except for the terms involving the z -
 244 component of the vector potential that can be dropped out in homogeneous domains. Here we
 245 show that, due to heterogeneity, all the components of the vector potential should be
 246 considered.

247 3.2 Homogeneous boundary conditions

248 The flow boundary conditions are derived in terms of vector potential. As it is shown in
 249 [Guerrero-Martínez et al. \[2016\]](#) and [Shao et al. \[2018\]](#), the flow boundary conditions can be
 250 written as follows:

$$\begin{aligned}
 \frac{\partial \psi_x}{\partial X} = \psi_Y = \psi_Z = 0, \quad \text{at } X = 0, 1 \\
 \frac{\partial \psi_Y}{\partial Y} = \psi_X = \psi_Z = 0, \quad \text{at } Y = 0, 1 \\
 \frac{\partial \psi_Z}{\partial Z} = \psi_X = \psi_Y = 0, \quad \text{at } Z = 0, 1
 \end{aligned} \quad (0)$$

252 Note that these homogeneous impervious boundary conditions for fluid flow are applicable
 253 for both configurations V-het and H-het. To derive homogeneous boundary conditions for
 254 heat transfer, we express the temperature boundary conditions in terms of dimensionless
 255 variables:

$$256 \quad \begin{cases} \mathcal{G} = f(Y), & \text{at } X = 0 \\ \mathcal{G} = 0, & \text{at } X = 1 \end{cases} \quad \frac{\partial \mathcal{G}}{\partial Y} = 0, \text{ at } Y = 0,1 \quad \frac{\partial \mathcal{G}}{\partial Z} = 0, \text{ at } Z = 0,1 \quad (0)$$

257 where $f(Y)$ is a constant $f(Y)=1$ for the V-het configuration, and defined as
 258 $f(Y) = (F(y) - T_c) / (T_h - T_c)$ for the H-het configuration. Further, we define the following
 259 change of variable:

$$260 \quad \theta = \mathcal{G} + (X - 1)f(Y) \quad (0)$$

261 Using the above equation, the boundary conditions in terms of the shifted dimensionless
 262 temperature θ become:

$$263 \quad \begin{aligned} \theta &= 0, & \text{at } X &= 0,1 \\ \frac{\partial \theta}{\partial Y} &= (X - 1)f'(Y), & \text{at } Y &= 0,1 \\ \frac{\partial \theta}{\partial Z} &= 0, & \text{at } Z &= 0,1 \end{aligned} \quad (0)$$

264 These temperature boundary conditions are periodic when the function $f(Y)$ satisfies the
 265 condition $f'(0) = f'(1) = 0$. For the V-het configuration, as $f(Y)=1$, this condition is
 266 satisfied in nature. For the H-het configuration, to meet this requirement, we select a
 267 particular function such that:

$$268 \quad f(Y) = \frac{1 + \cos(\pi Y)}{2} \quad (0)$$

269 Note that the presented method is not limited to this particular function. Any other function
 270 that leads to periodic boundary conditions is applicable. Substituting Eq. (14) into Eqs. (10)

271 and (11), one obtains the final system of governing equations in terms of the shifted
 272 temperature θ and vector potential components:

$$273 \quad \nabla^2 \psi_x + \frac{1}{k_p} \left(\frac{\partial k_p}{\partial Y} \left(\frac{\partial \psi_Y}{\partial X} - \frac{\partial \psi_X}{\partial Y} \right) - \frac{\partial k_p}{\partial Z} \left(\frac{\partial \psi_X}{\partial Z} - \frac{\partial \psi_Z}{\partial X} \right) \right) + Ra \frac{\partial \theta}{\partial Y} - Ra(X-1)f'(Y) = 0 \quad (0)$$

$$274 \quad \nabla^2 \psi_Y + \frac{1}{k_p} \frac{\partial k_p}{\partial Z} \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) - Ra \frac{\partial \theta}{\partial X} + Ra \cdot f(Y) = 0 \quad (0)$$

$$275 \quad \nabla^2 \psi_Z - \frac{1}{k_p} \frac{\partial k_p}{\partial Y} \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) = 0 \quad (0)$$

$$276 \quad \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) \frac{\partial \theta}{\partial X} + \left(\frac{\partial \psi_X}{\partial Z} - \frac{\partial \psi_Z}{\partial X} \right) \frac{\partial \theta}{\partial Y} + \left(\frac{\partial \psi_Y}{\partial X} - \frac{\partial \psi_X}{\partial Y} \right) \frac{\partial \theta}{\partial Z} - \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} + \frac{\partial^2 \theta}{\partial Z^2} \right) \\ - \left(\frac{\partial \psi_Z}{\partial Y} - \frac{\partial \psi_Y}{\partial Z} \right) f(Y) - \frac{\partial \psi_X}{\partial Z} (X-1)f'(Y) + (X-1)f''(Y) = 0 \quad (0)$$

277 3.3 The spectral system

278 The components of the vector potential ψ_x , ψ_Y , and ψ_Z , as well as the shifted temperature
 279 θ are expanded using infinite triple Fourier series that are truncated at given orders:

$$280 \quad \psi_x(X, Y, Z) = \sum_{i=0}^{Ni} \sum_{j=1}^{Nj} \sum_{k=1}^{Nk} A_{i,j,k} \cos(i\pi X) \sin(j\pi Y) \sin(k\pi Z) \quad (0)$$

$$281 \quad \psi_Y(X, Y, Z) = \sum_{l=1}^{Nl} \sum_{m=0}^{Nm} \sum_{n=1}^{Nn} B_{l,m,n} \sin(l\pi X) \cos(m\pi Y) \sin(n\pi Z) \quad (0)$$

$$282 \quad \psi_Z(X, Y, Z) = \sum_{d=1}^{Nd} \sum_{r=1}^{Nr} \sum_{s=0}^{Ns} C_{d,r,s} \sin(d\pi X) \sin(r\pi Y) \cos(s\pi Z) \quad (0)$$

$$283 \quad \theta(X, Y, Z) = \sum_{u=1}^{Nu} \sum_{v=0}^{Nv} \sum_{w=0}^{Nw} E_{u,v,w} \sin(u\pi X) \cos(v\pi Y) \cos(w\pi Z) \quad (0)$$

284 where Ni , Nj and Nk are the truncation orders for the vector potential component ψ_x in
 285 the X -, Y - and Z -directions. Similarly, Nl , Nm and Nn (resp. Nd , Nr and Ns) are that for
 286 ψ_Y (resp. ψ_Z). Nu , Nv and Nw are the truncation orders for the dimensionless temperature

287 θ . $A_{i,j,k}$, $B_{l,m,n}$, $C_{d,r,s}$ and $E_{u,v,w}$ are the Fourier series coefficients for the vector potential
 288 components ψ_X , ψ_Y , ψ_Z , and the temperature θ , respectively. It should be noted that all the
 289 above Fourier series expansions honor the periodic flow and temperature boundary conditions
 290 as shown in Eqs. (12) and (15).

291 The Fourier series expansions are substituted into Eqs. (17)-(20), and followed by the
 292 Galerkin treatment, where the resulted equations are multiplied, respectively, by the following
 293 trial functions that use Fourier modes:

$$\begin{aligned}
 \Lambda_{I,J,K}^{\psi_X} &= 8 \cos(I\pi X) \sin(J\pi Y) \sin(K\pi Z) & I = 0, \dots, Ni, J = 1, \dots, Nj, K = 1, \dots, Nk \\
 \Lambda_{L,M,N}^{\psi_Y} &= 8 \sin(L\pi X) \cos(M\pi Y) \sin(N\pi Z) & L = 1, \dots, Nl, M = 0, \dots, Nm, N = 1, \dots, Nn \\
 \Lambda_{D,R,S}^{\psi_Z} &= 8 \sin(D\pi X) \sin(R\pi Y) \cos(S\pi Z) & D = 1, \dots, Nd, R = 1, \dots, Nr, S = 0, \dots, Ns \\
 \Lambda_{U,V,W}^{\theta} &= 8 \sin(U\pi X) \cos(V\pi Y) \cos(W\pi Z) & U = 1, \dots, Nu, V = 0, \dots, Nv, W = 0, \dots, Nw
 \end{aligned}$$

295 The resulted equations are then integrated over the cubic domain. To allow an analytical
 296 evaluation of all the triple integrations arising from the FS method, we assume that
 297 permeability depends on space by means of an exponential function [Jiang et al., 2010; Fahs
 298 et al., 2015; Zhuang and Zhu, 2018]:

$$k_p(Y, Z) = k_0 e^{\sigma Y + \zeta Z} \quad (0)$$

300 where k_0 is the permeability at $Y = Z = 0$, and σ and ζ are the changing rate of $\ln(K_p)$ in
 301 the Y and Z direction, respectively. When $\sigma = \zeta = 0$, permeability is homogeneous over the
 302 domain. With $\sigma \neq 0$ and $\zeta = 0$, the porous medium is vertically stratified, and permeability
 303 varies in the Y direction, which is the case in the V-het configuration as shown in Fig. 1(a).
 304 While with $\sigma = 0$ and $\zeta \neq 0$, the porous medium is horizontally stratified, which is the case
 305 in the H-het configuration as shown in Fig. 1(b).

306 Eq. (25) allows us to integrate all Fourier integrals analytically, resulting in a system of
 307 nonlinear algebraic equations with the Fourier coefficients $A_{i,j,k}$, $B_{l,m,n}$, $C_{d,r,s}$, and $E_{u,v,w}$ as

308 unknowns. For the V-het configuration, the corresponding boundary condition and the
 309 permeability are set as $f(Y) = 1$ and $k_p = k_0 e^{\sigma Y}$, leading to the following residual equations:

$$\begin{aligned}
 RFX_{I,J,K} = & -\pi^2 \left(I^2 + \alpha_I J^2 + \alpha_I K^2 \right) A_{I,J,K} \\
 & - \sigma \left(\alpha_I \sum_{j=1}^{Nj} j \cdot A_{I,j,K} \Phi_{J,j} - I \cdot \sum_{m=0}^{Nm} B'_{I,m,K} \Phi_{J,m} \right) \\
 & - \frac{Ra_0}{\pi} \sum_{u=1}^{Nu} \sum_{v=0}^{Nv} \sum_{w=0}^{Nw} v \cdot E_{u,v,w} \Phi_{u,I} \Pi_{v,J} \Phi_{K,w} = 0 \\
 & (I = 0, \dots, Ni, J = 1, \dots, Nj, K = 1, \dots, Nk)
 \end{aligned} \tag{0}$$

$$\begin{aligned}
 RFY_{L,M,N} = & -\pi^2 \left(\alpha_M L^2 + M^2 + \alpha_M N^2 \right) B_{L,M,N} \\
 & - \frac{Ra_0}{\pi} \sum_{u=1}^{Nu} \sum_{v=0}^{Nv} \sum_{w=0}^{Nw} u \cdot E_{u,v,w} \Phi_{L,u} \Upsilon_{v,M} \Phi_{N,w} \\
 & + \frac{Ra_0}{\pi^2} \Phi_{L,0} \Upsilon_{M,0} \Phi_{N,0} = 0 \\
 & (L = 1, \dots, Nl, M = 0, \dots, Nm, N = 1, \dots, Nn)
 \end{aligned} \tag{0}$$

$$\begin{aligned}
 RFZ_{D,R,S} = & -\pi^2 C_{D,R,S} \left(\alpha_S D^2 + \alpha_S R^2 + S^2 \right) \\
 & + \sigma \left(S \cdot \sum_{m=0}^{Nm} B'_{D,m,S} \Phi_{R,m} - \alpha_S \cdot \sum_{r=0}^{Nr} r C_{D,r,S} \Phi_{R,r} \right) = 0 \\
 & (D = 1, \dots, Nd, R = 1, \dots, Nr, S = 0, \dots, Ns)
 \end{aligned} \tag{0}$$

$$\begin{aligned}
 RT_{U,V,W} = & \pi \left(\alpha_V \cdot W \cdot B'_{U,V,W} - \alpha_W \cdot V \cdot C'_{U,V,W} \right) - \pi^2 \left(\alpha_W \alpha_V U^2 + \alpha_W V^2 + \alpha_V W^2 \right) E_{U,V,W} \\
 & + \frac{\pi^2}{8} \sum_{u=1}^{Nu} \sum_{v=0}^{Nv} \sum_{w=0}^{Nw} E_{u,v,w} \left[\sum_{i=0}^{Ni} \sum_{j=1}^{Nj} \sum_{k=1}^{Nk} A_{i,j,k} \left(k \cdot v \cdot \xi_{i,u,U} \cdot \kappa_{j,v,V} \cdot \nu_{k,w,W} - j \cdot w \cdot \xi_{i,u,U} \cdot \nu_{j,v,V} \cdot \kappa_{k,w,W} \right) \right. \\
 & - \sum_{l=1}^{Nl} \sum_{m=0}^{Nm} \sum_{n=1}^{Nn} B_{l,m,n} \left(n \cdot u \cdot \kappa_{l,U,u} \cdot \zeta_{m,v,V} \cdot \nu_{n,w,W} - l \cdot w \cdot \xi_{l,u,U} \cdot \zeta_{m,v,V} \cdot \kappa_{n,w,W} \right) \\
 & \left. + \sum_{d=1}^{Nd} \sum_{r=1}^{Nr} \sum_{s=0}^{Ns} C_{d,r,s} \left(r \cdot u \cdot \kappa_{d,U,u} \cdot \nu_{r,v,V} \cdot \nu_{s,w,W} - d \cdot v \cdot \xi_{d,u,U} \cdot \kappa_{r,v,V} \cdot \zeta_{s,w,W} \right) \right] = 0 \\
 & (U = 1, \dots, Nu, V = 0, \dots, Nv, W = 0, \dots, Nw)
 \end{aligned} \tag{0}$$

314 where RFX , RFY , RFZ , and RT are the residuals corresponding to the three flow components
 315 and heat transfer equations, respectively. Ra_0 in Eqs. (26) and (27) is the thermal Rayleigh
 316 number at $Y=0$ and $Z=0$, defined as:

$$Ra_0 = \frac{\rho_c g k_0 H \beta \Delta T}{\mu \alpha} \tag{30}$$

318 For the V-het configuration, Ra_0 represents the Rayleigh number based on the permeability of
319 the lower layer ($Z=0$), while for the H-het configuration it is the Rayleigh number based on
320 the permeability of the vertical wall $Y=0$.

321 The residuals for the H-het configuration and the corresponding coefficients in these
322 equations are given in the Section S1 of Supplemental Material. We solve the system of
323 nonlinear equations using a nonlinear solver from the IMSL library based on the modified
324 Powell hybrid algorithm
(<https://docs.roguewave.com/imsl/fortran/7.1/html/fnlmath/index.html>), which is very
325 efficient. We include analytical evaluation of the Jacobian matrix to improve the performance
326 and convergence of the solver (see Supplemental Material Section S2). Besides, Eq. (29)
327 involves terms that have six overlapped summations, which are computationally expensive.
328 We simplify these terms from six to three nested summations, as in Shao et al. [2018], to
329 reduce computations. Indeed, this reformulation reduces CPU-time by 2 to 3 orders of
330 magnitude. Finally, parallel computing is implemented in these FG solutions to further reduce
331 the CPU time.

333 *3.4 Metrics for the assessment of convective flow, heat transfer and entropy generation*

334 The convective flow is assessed using the dimensionless velocity defined as follows:

$$335 \quad \mathbf{Q} = \frac{H}{\alpha} \mathbf{q} \quad (31)$$

336 The heat transfer performance is evaluated by the average Nusselt number that assesses the
337 heat diffusion across the boundary $X=0$ into the domain. The local Nusselt number is defined
338 by

$$339 \quad Nu = \frac{1}{g_{surf}} \left. \frac{\partial \mathcal{G}}{\partial X} \right|_{X=0} \quad (32)$$

340 where \mathcal{G}_{surf} is the imposed average temperature at the boundary $X=0$. For the V-het
 341 configuration, the average temperature at $X=0$ is $\mathcal{G}_{surf} = 1$. While for the H-het configuration,
 342 we have $\mathcal{G}_{surf} = \int_0^1 \int_0^1 f(Y) dXdZ = 1/2$. Using the Fourier series expansion of temperature, we
 343 obtain the local Nusselt number expressed by Fourier coefficients:

$$344 \quad Nu = \frac{\pi}{\mathcal{G}_{surf}} \sum_{u=1}^{Nu} \sum_{v=0}^{Nv} \sum_{w=0}^{Nw} u E_{u,v,w} \cos(v\pi Y) \cos(w\pi Z) - \frac{f(Y)}{\mathcal{G}_{surf}} \quad (33)$$

345 And the average Nusselt number is computed as follows:

$$346 \quad \overline{Nu} = \int_0^1 \int_0^1 Nu.dYdZ = \frac{\pi}{\mathcal{G}_{surf}} \sum_{u=1}^{Nu} u E_{u,0,0} - 1 \quad (34)$$

347 In the considered NC system, the associated entropy generation is due to heat transfer and
 348 Darcy dissipation. It can be computed by the evaluation of the time derivative of the
 349 temperature or concentration variance [Le borgne et al., 2010] under very specific transient
 350 conditions, but not for the steady-state case considered herein. Based on the local
 351 thermodynamic equilibrium of the linear transport theory, the local entropy generation for the
 352 3D natural convection is given by Baytaş [2000] and Ghachem et al. [2012]:

$$353 \quad S_E = \frac{\lambda_m}{T_c^2} \left[\left(\frac{\partial T}{\partial x} \right)^2 + \left(\frac{\partial T}{\partial y} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] + \frac{\mu}{T_c k_p} (q_x^2 + q_y^2 + q_z^2) \quad (35)$$

354 Note that the first term evaluates the tendency to temperature homogeneity, which is
 355 proportional to the time derivative of temperature variance in transient problems [Le borgne et
 356 al., 2010], while the second terms equal the viscous dissipation of energy, divided by T_c . The
 357 first term is especially relevant in solute mass transfer, where it is termed mixing rate, because
 358 mixing controls fast reactions, whose rate is limited by the rate at which reactants mix [De
 359 Simoni et al., 2005]. Using the change of variable, we obtain the local entropy generation in
 360 terms of dimensionless variables. And then we define the local entropy generation number as:

$$N_E = \left(\frac{\partial \theta}{\partial X} - f(Y) \right)^2 + \left(\frac{\partial \theta}{\partial Y} - (X-1)f'(Y) \right)^2 + \left(\frac{\partial \theta}{\partial Z} \right)^2 + \phi (Q_x^2 + Q_y^2 + Q_z^2) \quad (36)$$

N_T N_F

where Q_x , Q_y , and Q_z are dimensionless velocity components in the X, Y, and Z directions, respectively. And ϕ is the local irreversibility distribution ratio that depends on the variation of permeability in heterogeneous porous media:

$$\phi = \frac{\mu T_c \alpha^2}{\lambda_m (\Delta T)^2 k_p} \quad (37)$$

At $Y=0$ and $Z=0$, we have $\phi_0 = (\mu T_c \alpha^2) / (\lambda_m (\Delta T)^2 k_0)$. It is noted that the value of ϕ_0 is dependent on the thermal Rayleigh number (Ra_0). In this work, as in Baytaş [2000], we take:

$$\phi_0 = \frac{10}{Ra_0} \quad (38)$$

In Eq. (36), N_T and N_F represent the irreversibility caused by mixing (dimensionless mixing rate) and Darcy dissipation (dimensionless viscous dissipation), respectively. Based on these, the Bejan number $Be = N_T / N_E$ that denotes the ratio of heat transfer irreversibility to the local entropy generation is defined. If the Bejan number is over 0.5, it implies that the irreversibility due to heat transfer plays a more important role in the entropy generation; otherwise, the irreversibility caused by fluid flow makes the dominant contribution. Furthermore, to assess the overall entropy generation in the domain, the total entropy generation number and the average Bejan number in the cubic enclosure are computed by:

$$N_{tot} = \int_0^1 \int_0^1 \int_0^1 N_E dXdYdZ \quad (39)$$

$$\overline{Be} = \int_0^1 \int_0^1 \int_0^1 Be dXdYdZ \quad (40)$$

4 Results and discussion

380 Three targets are discussed in this section. As a new code has been developed for the FS
 381 solution, we first verify the correctness of this code by comparison against finite element (FE)
 382 solutions obtained using COMSOL Multiphysics. Secondly, we present high-quality data that
 383 can be used as reference solutions for benchmarking numerical models dealing with NC,
 384 mixing, and entropy generation in heterogeneous porous domains. Then, taking advantage of
 385 the developed FS solution, we investigate the influence of heterogeneity and Rayleigh number
 386 on NC and processes irreversibility, and we evaluate the significance of the 3D processes by
 387 comparing 2D and 3D simulations.

388 As can be deduced from the dimensionless governing equations, NC processes and associated
 389 entropy generation are controlled by three parameters: the local Rayleigh number Ra_0 , the
 390 heterogeneity structure (parameterized here in terms of σ for the V-het configuration and ζ
 391 for the H-het configuration) and the local irreversibility distribution ratio (ϕ_0). The latter is
 392 linked to Ra_0 as in Eq. (38). For an adequate analysis, in our investigation, we replace Ra_0 by
 393 the effective large-scale Rayleigh number defined based on the average permeability as
 394 follows:

$$395 \quad \overline{Ra} = \frac{\rho_c g \overline{k_p} H \beta \Delta T}{\mu \alpha} \quad (41)$$

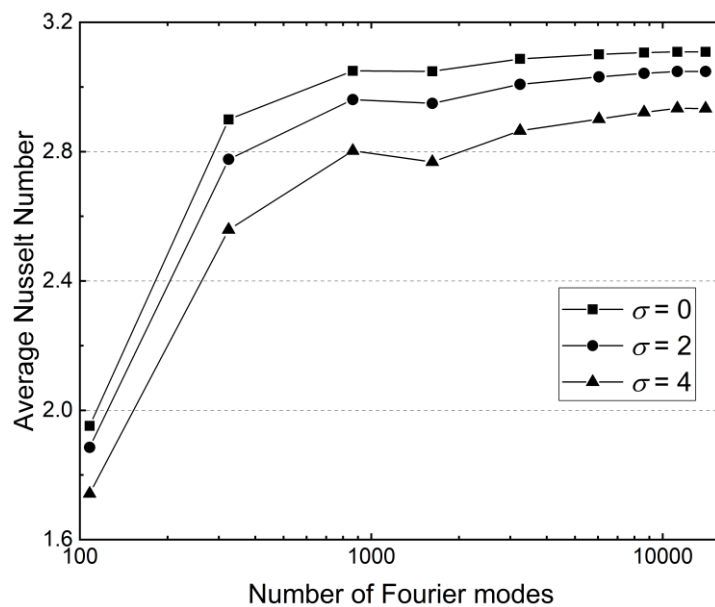
396 where $\overline{k_p} = \int_0^1 \int_0^1 \int_0^1 k_p(Y, Z) dXdYdZ$ is the large-scale average permeability in the cubic
 397 enclosure. The choice is non-trivial, and the effective value of permeability (i.e., the value of
 398 homogeneous permeability allowing the same flux through the medium as the actual
 399 permeability) has been the subject of research in the oil and hydrology literature [Noetinger,
 400 1994; Renard and de Marsily, 1997; Sanchez-Vila et al., 2006]. What has been found is that
 401 the appropriate averaging of permeability depends on the flow dimension. In 1D, the effective
 402 permeability is the harmonic average (k_H). In 2D, the effective permeability is the geometric

403 average (k_G). In 3D, the effective permeability is the 1/3 power average ($k_{1/3}$). The arithmetic
 404 average adopted here (k_A) is only appropriate for mathematically ideal infinite dimensions.
 405 When heterogeneity is large, these averages can be very different. Herein we analyze cases
 406 with $\sigma = 2$, where the largest permeability is 7.4 larger than the smallest one and the above
 407 four averages (k_A , $k_{1/3}$, k_G , and k_H) equal 3.2, 2.9, 2.7, and 2.3, respectively, which are not
 408 significantly different. Then we analyze cases with $\sigma = 4$, where the largest permeability is
 409 54.6 larger than the smallest one, and the above averages now equal 13.4, 9.2, 7.4, and 4.1,
 410 which are not dramatically different either. For a given heterogeneity, the large-scale
 411 Rayleigh number is proportional to the adopted effective permeability. As we shall see, when
 412 the large-scale Rayleigh number (\overline{Ra}) is constant, entropy indicators remain virtually
 413 unchanged when the heterogeneity rate is changed. However, they would increase
 414 dramatically if we had adopted any other average for effective permeability, because k_0 would
 415 have to be increased in order to maintain the large-scale Rayleigh number unchanged,
 416 Thus in all our simulations, we consider the large-scale Rayleigh number (\overline{Ra}) and the rate of
 417 heterogeneity (σ or ζ) as primary parameters controlling physical processes. Based on these
 418 parameters, we evaluate the parameters such as the local Rayleigh number (Ra_0) and the local
 419 irreversibility distribution ratio (ϕ_0).

420 *4.1 Verification of the FS solution*

421 The number of Fourier modes may affect the accuracy of the FS solutions. We adopt the
 422 technique developed by [Fahs et al. \[2015\]](#) to determine the appropriate Fourier modes leading
 423 to stable solutions. This technique proceeds by increasing the number of Fourier modes until
 424 reaching stable solutions. For the sake of simplicity, we adopt the same number of Fourier
 425 coefficients for ψ_x , ψ_y , ψ_z , and θ , that is $NX=Ni+1=Nl=Nd=Nu$, $NY=Nj=Nm+1=Nr=Nv+1$,
 426 and $NZ=Nk=Nn=Ns+1=Nw+1$. Accordingly, several levels of truncations orders with

427 increasing values of NX , NY , and NZ are tested and the stability is assessed based on the
 428 sensitivity of the average Nusselt number (\overline{Nu}) to the Fourier modes. Fig. 2 exemplifies the
 429 convergence behavior of the FS solution. It shows the variation of \overline{Nu} versus the total number
 430 of Fourier modes for three test cases of the V-het configuration, with $\overline{Ra} = 100$ and three
 431 levels of heterogeneity. It is found that for $\sigma = 0, 2$, and 4 , the converged FS solutions with
 432 stable \overline{Nu} values are obtained with 6,084 ($NX=24$, $NY=3$, and $NZ=21$), 8,640 ($NX=30$, $NY=3$,
 433 and $NZ=24$), and 11,232 ($NX=39$, $NY=3$, and $NZ=24$) Fourier modes, respectively. Typically,
 434 the increase of the rate of heterogeneity leads to a higher local Rayleigh number, and thus
 435 enhances the thermal convection at high permeable zones. For instance, with $\overline{Ra} = 100$ and
 436 $\sigma = 4$, the maximum local Rayleigh number in the domain can reach more than 400. In
 437 convection-dominant problems, a large number of Fourier modes is usually required to avoid
 438 Gibbs phenomenon and to obtain oscillation-free results [Peyret, 2002]. We should mention
 439 that the most important truncation order controlling oscillations is NX . Similar behaviours of
 440 the FS solution have been observed for the H-het configuration but they are not presented here
 441 for the sake of brevity.



443

444 **Fig. 2.** Example of the convergence of the FS solutions: Variation of the average Nusselt
 445 number (\overline{Nu}) versus the total number of Fourier modes for the V-het configuration (vertical
 446 heterogeneity) at $\overline{Ra} = 100$.
 447

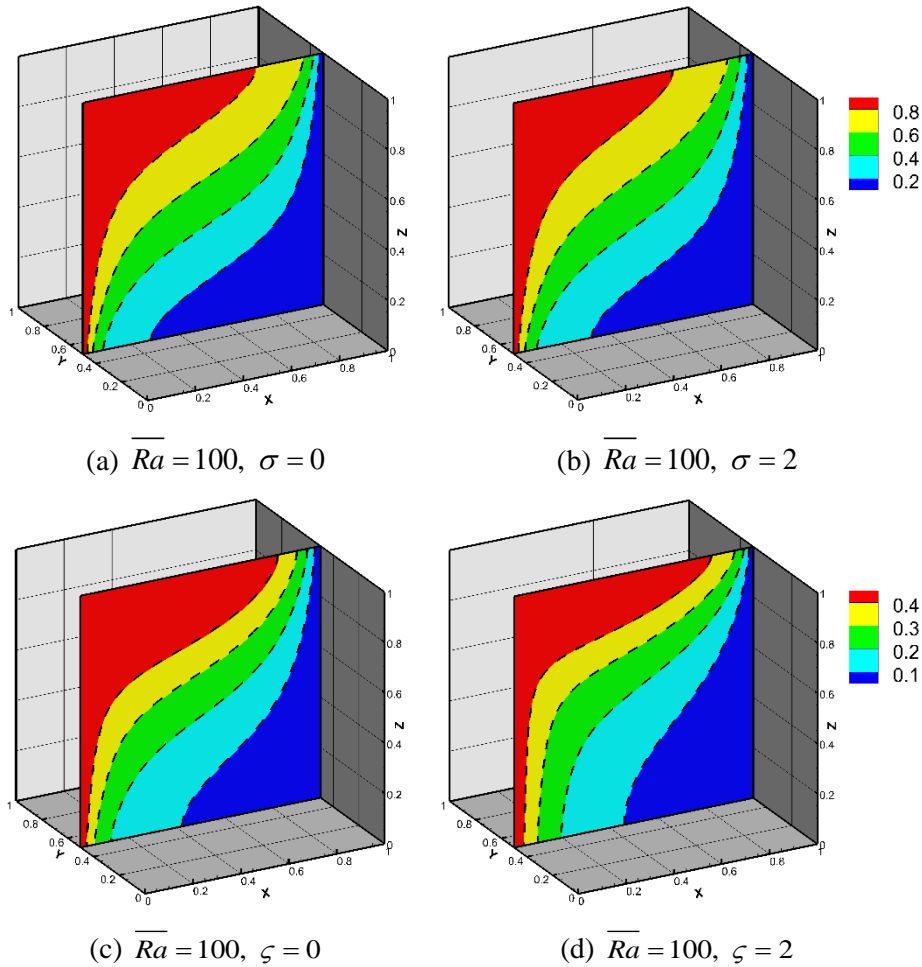
448 To further verify the FS solutions, a FE analysis is performed for some test cases using
 449 COMSOL Multiphysics. We checked relatively simple cases, dealing with $\overline{Ra} = 100$ and low
 450 rates of heterogeneity ($\sigma = 0$ and 2 for the V-het configuration and $\zeta = 0, 2$ for the H-het
 451 configuration), in order to facilitate convergence and to avoid numerical artifacts in the FE
 452 solutions that could affect the comparisons. A grid dependence test is conducted for each case
 453 using different levels of grid refinement in COMSOL. The FE computations are challenging
 454 because the gridding effect is important. The mesh-independent solutions have been obtained
 455 with a computational mesh of about 80K nodes in the homogeneous cases ($\sigma = 0$ or $\zeta = 0$)
 456 and 310K nodes for the heterogeneous cases ($\sigma = 2$ or $\zeta = 2$). The temperature field at the
 457 vertical slice $Y=0.5$ obtained from FS and FE solutions for these test cases are plotted in Fig.
 458 3. Table 2 lists the converged results of the average Nusselt number. From Fig. 3 and Table 2,
 459 it is observed that FS solutions show excellent agreement with FE solutions at various
 460 parameters, which indicates the correctness of the code developed for the FS solutions and
 461 gives confidence in the correctness of the developed COMSOL model. It is relevant to
 462 mention that while similar accuracy are obtained for these test cases with both solutions, the
 463 FS solution is significantly more efficient as it requires fewer degrees of freedom than the FE
 464 solution. For instance, in the V-het configuration ($\sigma = 2$), the FS solution is obtained with
 465 8,640 Fourier modes while the FE solution requires a computational mesh of 310K nodes
 466 involving more than 620K degrees of freedom.

467

468 **Table 2.** Comparison between the FS and FE solutions: The average Nusselt number

\overline{Nu}	Configuration V-het		Configuration H-het	
	$\sigma = 0$	$\sigma = 2$	$\zeta = 0$	$\zeta = 2$
FS solution	3.101	3.048	2.474	2.357

FE solution	3.073	2.981	2.456	2.343
-------------	-------	-------	-------	-------



470

471 **Fig. 3.** Comparison between the FS (colored map) and FE (dashed lines) solutions: The main
 472 isotherms at the vertical slice $Y=0.5$ for the configurations V-het (top) and H-het (bottom).

473

474 4.2 Reference solutions for code benchmarking: NC and entropy generation

475 The problem of NC in a porous enclosure is accepted as a common benchmark for numerical

476 codes. Different solutions of this problem have been obtained based on a variety of numerical

477 methods (see Fahs et al. [2015] and reference therein). Comparison between existing solutions

478 is widely used to validate and assess new developed numerical schemes and to help modelers

479 in handling codes interfaces and in data processing. Due to computation limitations, the

480 existing solutions are restricted to 2D. Even in 2D, the numerical accuracy of the entropy

481 generation is not well discussed, which can be significant because it requires a delicate post-

482 processing procedure based on the reconstruction of thermal and fluid fluxes. Here, taking
483 advantage of the accuracy and performance of the developed FS method, we provide
484 reference solutions that could be useful for benchmarking codes dealing with NC in porous
485 domains and associated entropy generation. The first set of solutions deal with low large-scale
486 Rayleigh number ($\overline{Ra} = 10$) with different rates of heterogeneity ($\sigma = 0, 2$ and 4 for the V-
487 het configuration and $\zeta = 0, 2$ and 4 for the H-het configuration). These cases are relatively
488 simple from the computational point of view as they deal with a low Rayleigh number. They
489 are useful for codes validations but not appropriate for inter-codes comparison. A relevant
490 benchmark problem for comparing numerical methods should be able to make clear
491 distinctions between the compared methods. Thus, we present solutions for cases dealing with
492 relatively high Rayleigh number and a high rate of heterogeneity. For such cases, it is well-
493 known that numerical schemes may lead to errors with clear grid-based artifacts. Accurate
494 solutions of such cases represent a major challenge for finite-element simulations.
495 Heterogeneity compounds the challenge as an accurate velocity field in heterogenous porous
496 media requires appropriate numerical schemes [Younes et al. 2013]. Thus, we present a
497 second set of solutions for cases dealing with $\overline{Ra} = 200$ and $\sigma = 0, 2$ and 4 (for the V-het
498 configuration) and $\zeta = 0, 2$ and 4 (for the H-het configuration).

499 We provide several quantitative indicators related to heat transfer and entropy generation. The
500 quantitative indicators facilitate inter-code comparison as they are more for comparison than
501 visual inspection of isotherms [Prasad and Simmons, 2005]. We use the average Nusselt
502 number as a metric of heat transfer processes, and the total entropy generation as well as the
503 average Bejan numbers to assess entropy generation. All these metrics are calculated without
504 any approximation based on the Fourier series. The results for all test cases are summarized in
505 Table 3. This table provides high-quality data that could be used as references for
506 benchmarking codes dealing with NC and related entropy generation.

507

508 **Table 3.** Quantitative indicators for benchmarking: average Nusselt number (\overline{Nu}), total
 509 entropy generation number (N_{tot}) and the average Bejan number (\overline{Be}).

	Configuration V-het					
	$\overline{Ra} = 10$			$\overline{Ra} = 200$		
	$\sigma = 0$	$\sigma = 2$	$\sigma = 4$	$\sigma = 0$	$\sigma = 2$	$\sigma = 4$
\overline{Nu}	1.079	1.090	1.111	4.936	4.751	4.218
N_{tot}	4.493	4.493	4.529	40.729	39.485	46.349
\overline{Be}	0.319	0.356	0.453	0.164	0.166	0.170
	Configuration H-het					
	$\overline{Ra} = 10$			$\overline{Ra} = 200$		
	$\zeta = 0$	$\zeta = 2$	$\zeta = 4$	$\zeta = 0$	$\zeta = 2$	$\zeta = 4$
\overline{Nu}	1.042	1.037	1.027	3.921	3.737	3.295
N_{tot}	2.419	2.238	1.866	21.205	18.949	15.243
\overline{Be}	0.316	0.328	0.379	0.151	0.143	0.138

510

511

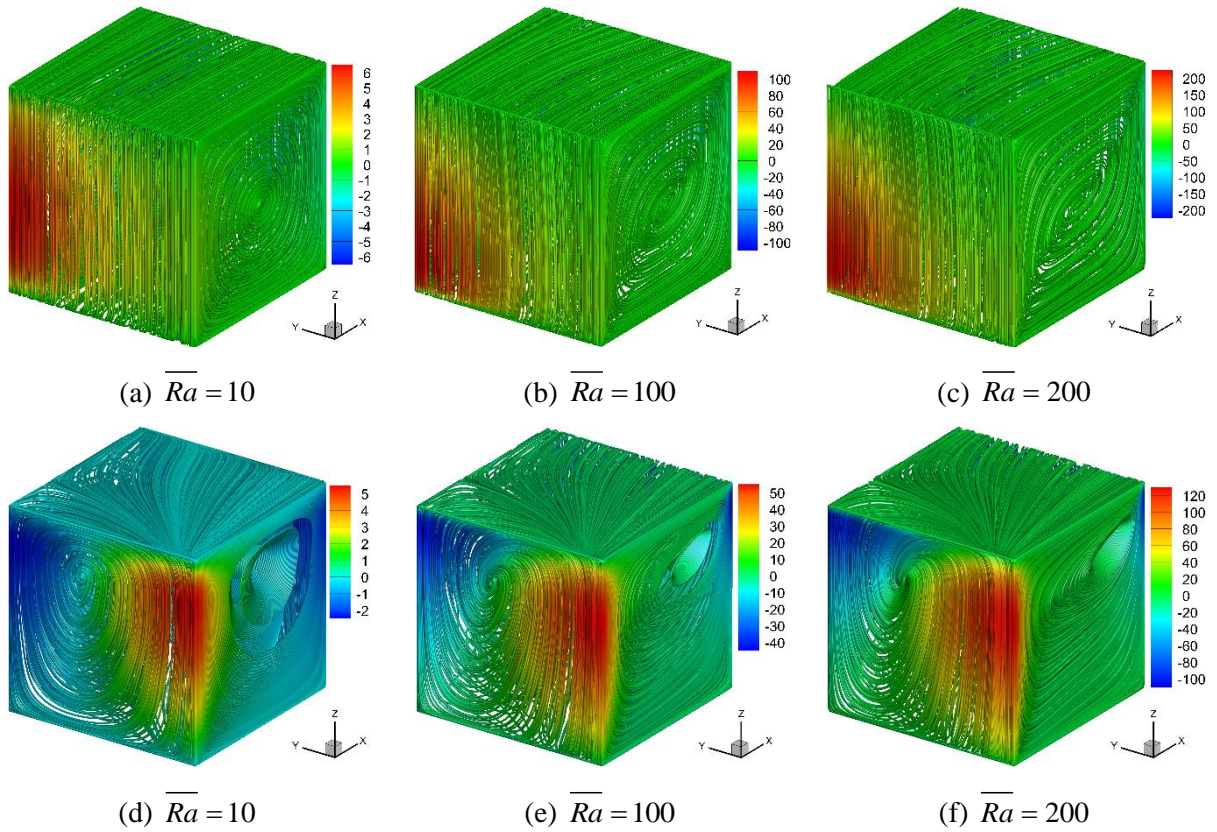
512 *4.3 Effect of large-scale thermal Rayleigh number on NC and entropy generation in*
 513 *heterogeneous domains*

514 The Rayleigh number is the main parameter controlling NC processes. In homogeneous
 515 domains, the effect of this number on convective flow, heat fluxes and processes
 516 irreversibility is a common topic in literature. In this work, we suggest the use of the large-
 517 scale number (\overline{Ra}) as the controlling parameter in heterogeneous domain. This section aims
 518 at investigating the effect of this new suggested \overline{Ra} on NC and entropy generation in
 519 heterogeneous domain. To this end, we analyze the configurations V-het ($\sigma = 2$) and H-het
 520 ($\zeta = 2$) with varied large-scale Rayleigh numbers ($\overline{Ra} = 10, 100, \text{ and } 200$).

521 To understand the flow structure, we plot in Fig. 4 the stream-tubes highlighted with the
 522 Darcy's vertical velocity component (Q_z). For the V-het configuration (Figs. 4a-4c), one
 523 main convective vortex (torus-like convection cell) occurs in the domain around the central
 524 axis of symmetry parallel to the Y-axis. The vertical velocity component (color scale)
 525 indicates a clockwise rotating flow, as expected (hot water flows up the hot face, $X=0$, and

526 down the cold face, $X=1$, with faster velocity near the back face, $Y=1$, where permeability is
527 the largest). The shape and orientation of the vortex depend on the large-scale Rayleigh
528 number. From this point of view, the latter has a similar effect as the local Rayleigh number in
529 homogeneous domain. While the vortex is centric and axially symmetrical for $\overline{Ra} = 10$, it
530 becomes diagonally-oriented and loses its central orientation when the large-scale Rayleigh
531 number is increased. At a constant heterogeneity rate (σ), the increase of the large-scale
532 Rayleigh number can be interpreted as an increase of permeability everywhere in the domain.
533 Thus, the convective flow becomes faster (notice the colour scale in Figs. 4a, b and c), the
534 thermal boundary around the vertical hot and cold walls shrinks and the zone of high velocity
535 moves down, as it can be observed in Figs. 4b and 4c.

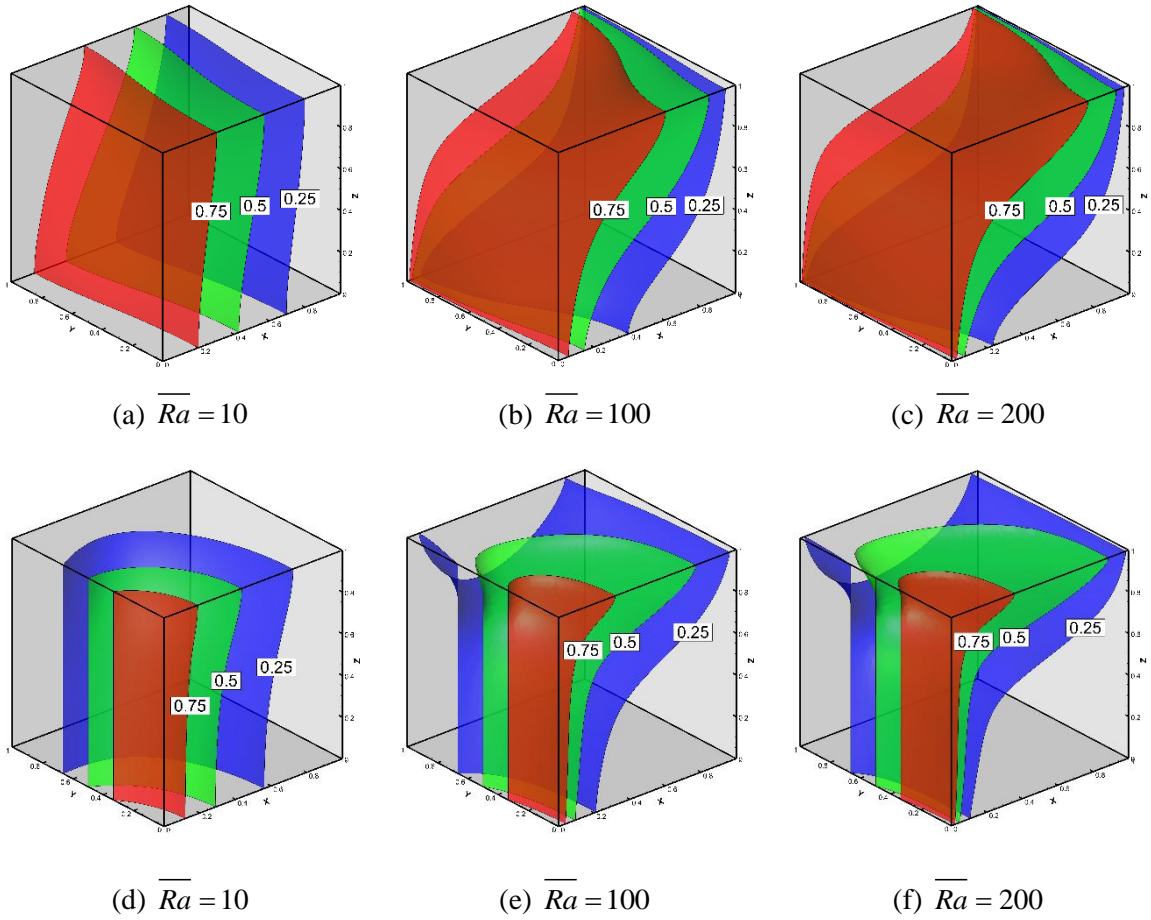
536 For the H-het configuration (Figs. 4d-4f), the flow structure is complex (recall Fig. 1b that
537 temperature is prescribed as a variable at the $X=0$ face). The main flow structure has the shape
538 of a convergent-divergent spiral vortex with a curved axis oriented from the vertical plane
539 $X=0$ to the vertical plane $Y=0$. The vortex structure of the flow is related to both crossed
540 temperature gradients occurring in the domain. The first gradient is generated by the
541 temperature difference between the hot and cold walls (oriented along the X -axis), while the
542 second gradient is related to the variable temperature imposed at the hot wall (oriented along
543 the Y -axis). As for the V-het configuration, the large-scale Rayleigh number affects the flow
544 structure and mainly the location of the vortex at the vertical plane $Y=0$. The location of the
545 vortex at the vertical plane $X=0$ is slightly sensitive to \overline{Ra} . This makes sense as the origin of
546 the vortex shape at $X=0$ is the temperature gradient imposed as a boundary condition and
547 independent on \overline{Ra} . For both configurations V-het and H-het, the scales of Q_z shows a
548 significant acceleration of the rotating flow with the increase of \overline{Ra} .



549 **Fig. 4.** Effect of large-scale Rayleigh number (\overline{Ra}) on convective flow: Stream-tubes
 550 highlighted with the vertical velocity component (Q_z) for the V-het configuration ($\sigma = 2$,
 551 top) and H-het ($\zeta = 2$, bottom), respectively.

552
 553 Fig. 5 depicts the isothermal surfaces for each test case. Buoyancy causes the top face to be
 554 warmer than the bottom face. However, the two configurations exhibit completely different
 555 temperature fields owing to the distinct layouts of heterogeneity and different boundary
 556 conditions. At low \overline{Ra} , the heat transfer processes are mainly conductive. The isothermal
 557 surfaces are almost vertical. With the increase of \overline{Ra} , the isothermal surfaces become more
 558 distorted inside the enclosure as they follow the flow structure. The transition zone becomes
 559 narrower close to the hot boundary (at $X=0$) because convective heat transfer is enhanced.

560

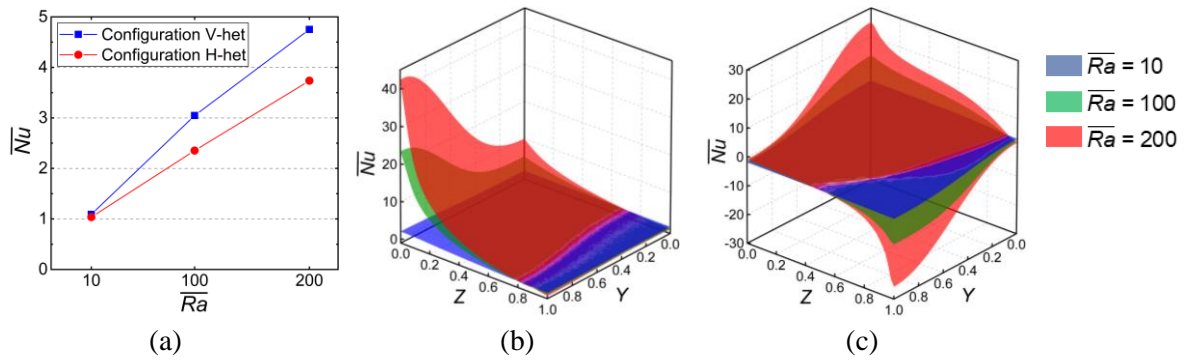


561 **Fig. 5.** Effect of large-scale Rayleigh number (\overline{Ra}) on temperature distribution: Main
 562 temperature iso-surfaces for the configuration V-het ($\sigma = 2$, top) and H-het ($\zeta = 2$, bottom),
 563 respectively.
 564

565 The variation of the average Nusselt number with respect to \overline{Ra} is given in Fig. 6a. This
 566 figure indicates that \overline{Nu} increases with \overline{Ra} , as the buoyancy-induced flow enhances the
 567 diffusive heat transfer across the boundary. At the same level of large-scale Rayleigh number
 568 and heterogeneity rate, vertical heterogeneity leads to more heat transfer to the domain than
 569 horizontal heterogeneity. The space distribution of the heat flux through the hot wall is also
 570 investigated using the local Nusselt number as in Figs. 6b and 6c. It is clear that, for the V-het
 571 configuration, at a low Rayleigh regime, the heat flux to the domain is uniformly distributed.
 572 The increase of \overline{Ra} enhances the heat flux locally in the bottom part of the hot wall (near
 573 $Z=0$), particularly in the high permeable zone. The heat flux at the upper part of the wall (near

574 $Z=1$) is slightly sensitive to \overline{Ra} . For the H-het configuration, we can observe negative local
575 Nusselt numbers, indicating heat losses in some parts of the wall. This is due to the variable
576 temperature imposed at the hot wall. In these parts, due to convective flow in the Y direction
577 (caused by the variable temperature), the temperature of the fluid in the thermal boundary
578 layer becomes higher than the imposed temperature, leading to a heat flux from the domain to
579 the hot wall. The largest heat flux to the domain is observed at the bottom corner ($Y=Z=0$).

580



581 **Fig. 6.** Effects of the large-scale Rayleigh number (\overline{Ra}) on heat flux through the hot wall: (a)
582 the average Nusselt number, (b) and (c) maps of local Nusselt number of the hot wall for the
583 configurations V-het ($\sigma = 2$) and H-het ($\zeta = 2$), respectively.

584

585

586 Fig. 7 depicts the local entropy generation number N_E for both configurations V-het and H-
587 het with $\overline{Ra} = 10, 100, \text{ and } 200$. For the V-het configuration, in the case of low \overline{Ra} (Fig. 7a),
588 two zones of high entropy generation can be observed. The first one is located within the
589 thermal boundary layer near the hot and cold walls, in the high permeable area (toward $Y=1$).
590 In this zone, the high permeability leads to a high fluid circulation, which causes
591 irreversibility due to viscous dissipation. The fact that the geometry of this high entropy
592 generation zone resembles the geometry of the high-velocity zone (red in Fig. 4) points that
593 viscous dissipation, rather than mixing, is the main entropy generation process. Mixing only
594 displays in enlarging the high entropy generation towards the bottom of the $X=0$ face, where
595 temperature gradients are highest (see Fig. 5). For low Rayleigh number, a second zone of

596 high entropy generation is located near the top ($Z=1$) where velocity is high due to the
 597 heterogeneity. This zone is displaced to the back ($X=1$) when Rayleigh number increases
 598 which causes a severe increase in temperature gradients and thus to mixing between hot and
 599 cold fluids. The temperature gradient in this zone is relatively high due to mixing. Thus
 600 entropy generation in this zone is mainly related to the conduction effect. When \overline{Ra} is
 601 increased (Figs. 7b and 7c), the thermal boundary layer shrinks, and the fluid circulation
 602 increases. But, overall, entropy generation due to flow dominates, and the maximum local
 603 entropy generation appears within the thermal boundary layer near the hot and cold walls at
 604 $X=0$ and $X=1$ and increases along the Y axis from $Y=0$ and $Y=1$, as the gradient of temperature
 605 and the velocity field are intensified locally due to the heterogeneity of porous medium. For
 606 the H-het configuration, the zone of high entropy generation is located just near the hot wall,
 607 in contrast to the V-het configuration where high entropy generation is observed near both hot
 608 and cold walls. This is related to the boundary conditions. Near the hot wall, there is a thermal
 609 gradient related to the imposed variable temperature and the temperature difference with the
 610 cold wall. Thus entropy generation due to heat transfer at the hot side ($Y=0$) of the hot wall
 611 ($X=0$) is more important than that at the cold wall. Note also that entropy generation is more
 612 pronounced at the top surface than at the bottom surface, where permeability is smallest.

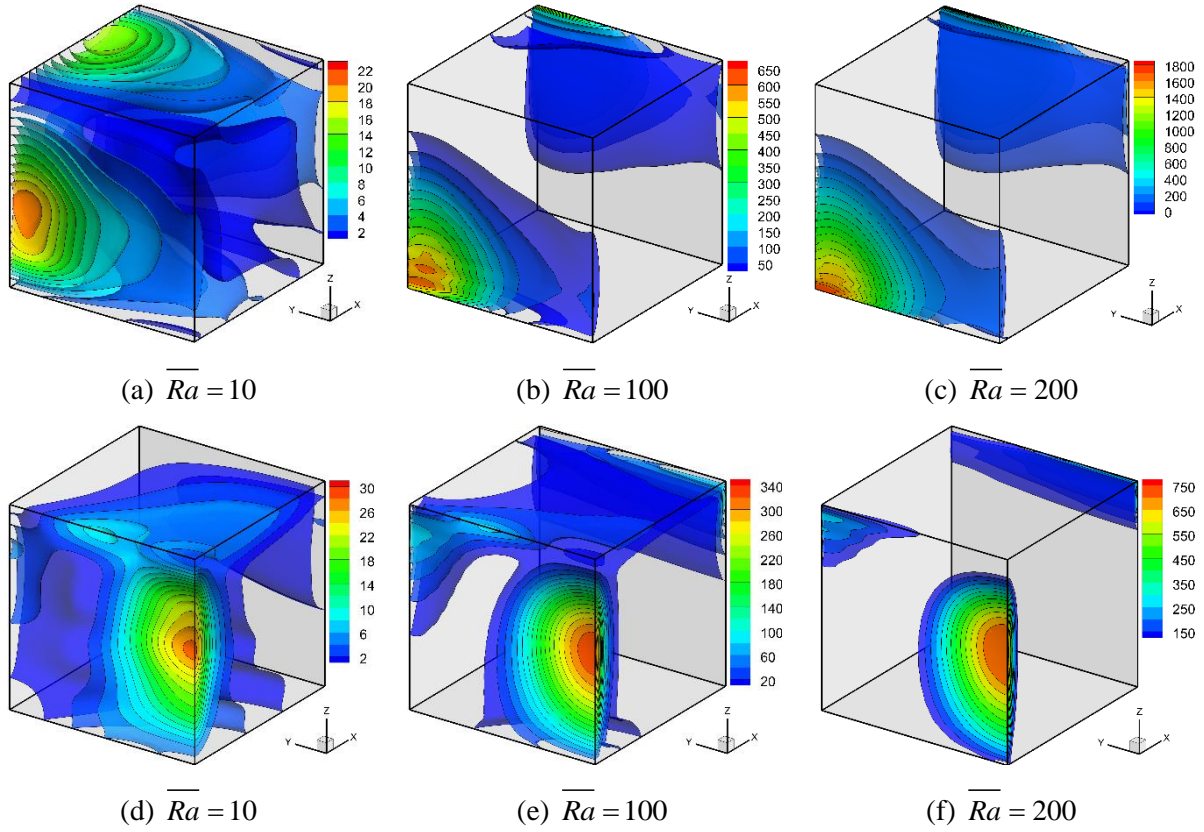
613 Fig.8 depicts the variation of total entropy generation number (N_{tot}), the total mixing rate (N_T),
 614 and the average Bejan number (\overline{Be}) as a function of the large-scale Rayleigh number.
 615 For both configurations, V-het and H-het, the total entropy generation number increases
 616 significantly with \overline{Ra} , as the higher \overline{Ra} leads to an enhancement of fluid flow and
 617 convective heat transfer (Fig. 8a). Also in both configurations, all the average Bejan numbers
 618 are far below 0.5, indicating that the irreversibility due to fluid flow makes the major
 619 contribution on the total entropy generation. Besides, \overline{Be} decreases with the increase of \overline{Ra} .

620 This indicates that fluid flow irreversibility becomes more significant with the increase of \overline{Ra}

621 .

622

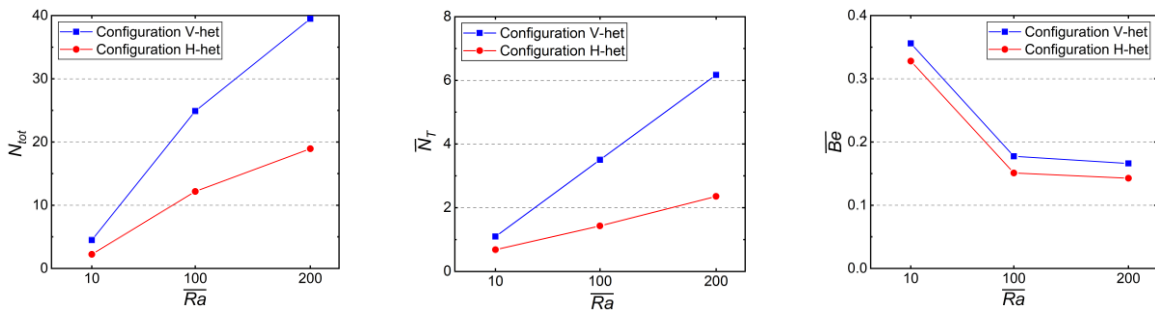
623



624 **Fig. 7.** Effect of large-scale Rayleigh number (\overline{Ra}) on entropy generation: Iso-surfaces of
 625 local entropy generation number (N_E) for the configuration V-het ($\sigma = 2$, top) and H-het (
 626 $\zeta = 2$, bottom), respectively.

627

628



629 **Fig. 8.** Effect of large-scale Rayleigh number (\overline{Ra}) on entropy generation: The total entropy
 630 generation number (N_{tot} , left), the total mixing rate (N_T , center), and the average Bejan
 631 number (\overline{Be} , right) for the configuration V-het ($\sigma = 2$) and H-het ($\zeta = 2$), respectively.

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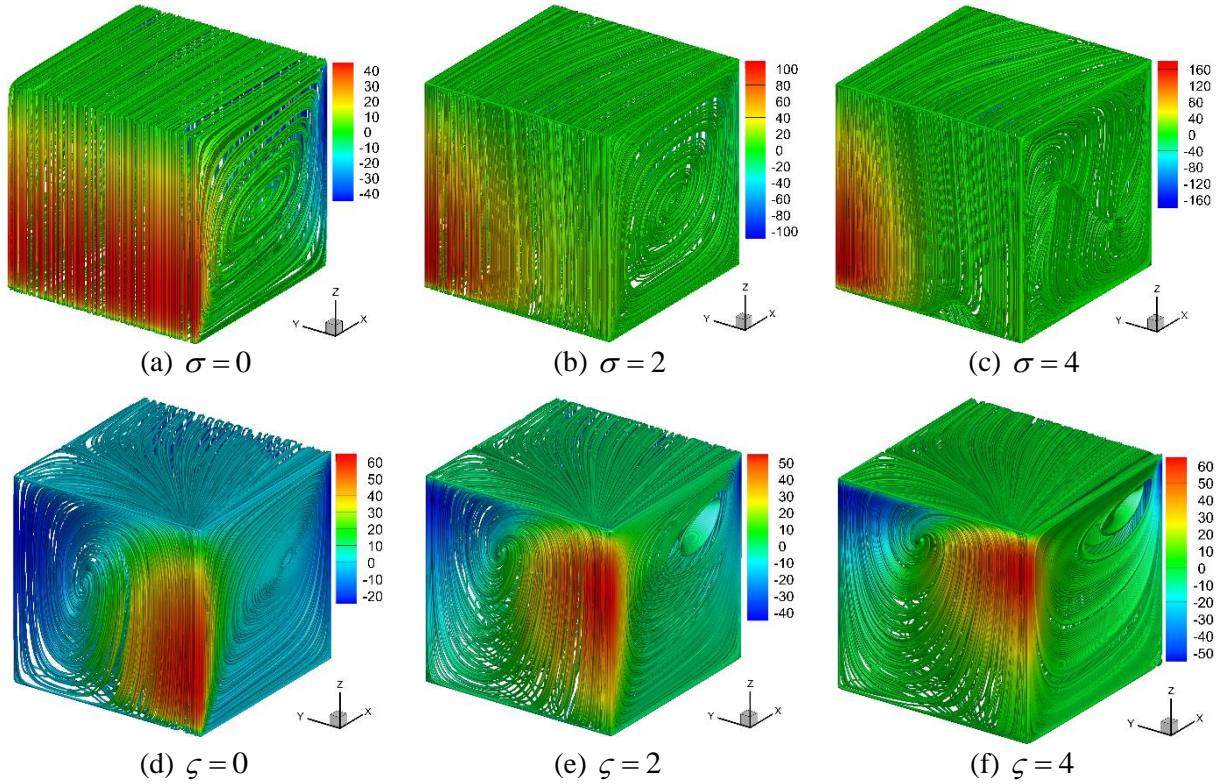
4.4 Influence of heterogeneity

639 To investigate the effect of varying heterogeneity on the 3D natural convection and entropy
640 generation, we fix the large-scale Rayleigh number at $\overline{Ra}=100$, and vary the rate of
641 heterogeneity from 0 to 4. Fig. 9 shows the stream-tubes highlighted with the Darcy's vertical
642 velocity component (Q_z) for the rate of heterogeneity varying from 0 to 4. We recall that, at a
643 constant large-scale Rayleigh number, the increase of the rate of heterogeneity, for the
644 configuration V-het (resp. H-het) corresponds to higher permeability around the vertical plane
645 $Y=1$ (resp. top surface) and lower permeability near the vertical wall $Y=0$ (resp. bottom
646 surface), so that the arithmetic average of permeability is the same for the the three rates. For
647 the V-het configuration (Figs. 9a-9c), increasing heterogeneity enhances fluid flow locally
648 and raises the maximum vertical velocity component. The region of maximum Q_z moves
649 toward the corner near $Y=1$ as the rate of heterogeneity increases, because increasing
650 heterogeneity induces an increase of the local Rayleigh number near $Y=1$, and a decrease near
651 $Y=0$. The flow structure for $\sigma=0$ (homogeneous case, when the flow structure is 2D) and
652 $\sigma=2$ are quite similar, except for the increase of vertical flux near $Y=1$ at the front ($X=0$)
653 face. However, for the high rate of heterogeneity, we can observe two vortices in the zone of
654 low permeability.

655 For the H-het configuration (Figs. 9d-9f) the region of maximum velocity moves upward with
656 the increase of the level of heterogeneity, as expected. However, the value of maximum
657 velocity for this configuration is only slightly influenced by the variation of heterogeneity
658 rate. In contrast to the V-het configuration, the flow structure is affected by the rate of
659 heterogeneity, as it can be observed in Figs. 9d-9f, where the location of the vortices at the

660 planes $X=0$ and $Y=0$ are moving towards the high permeable zones when the rate of
 661 heterogeneity is increased.

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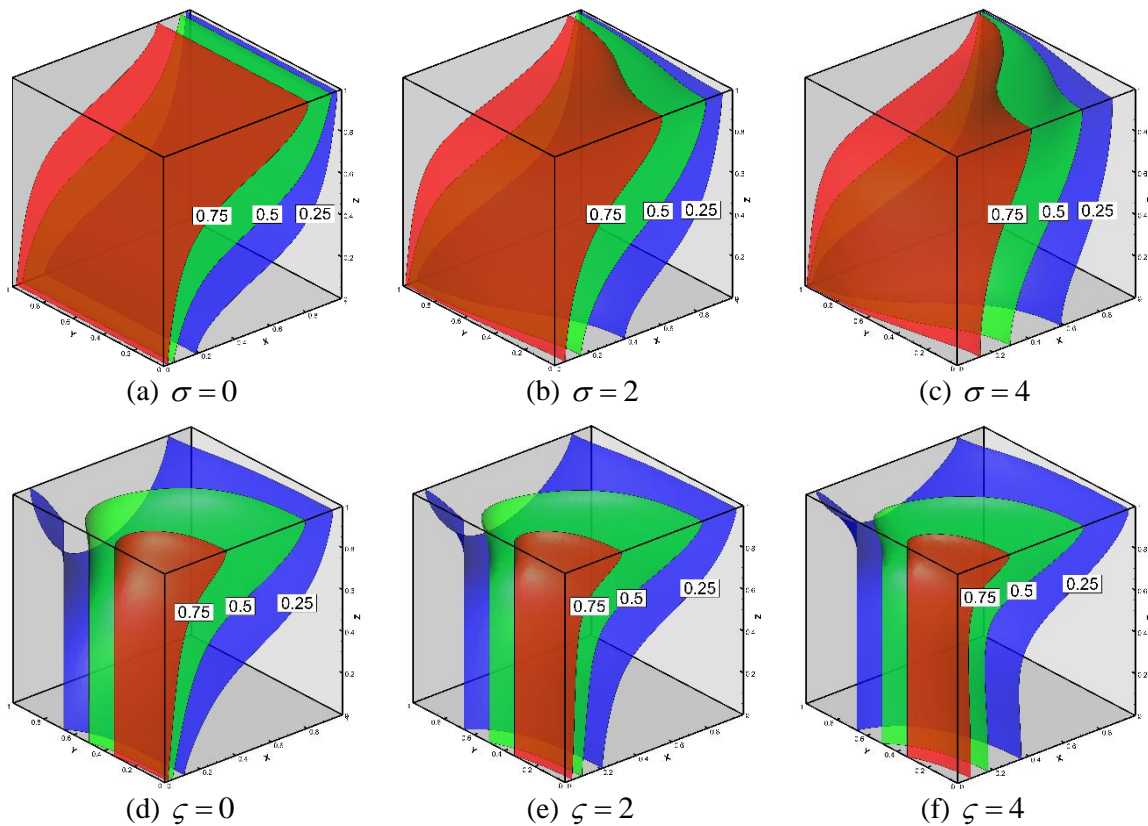
664 **Fig. 9.** Effect of heterogeneity on convective flow: Stream-tubes highlighted with the vertical
 665 velocity component (Q_z) for the configuration V-het (top) and H-het (bottom) for $\overline{Ra} = 100$.

666

667 The isothermal surfaces for both configurations are plotted in Fig. 10. For the V-het
 668 configuration, when the level of heterogeneity is $\sigma = 0$, the porous medium is homogeneous,
 669 resulting in a quasi 2D problem. The isothermal surfaces, shown in Fig. 10a, exhibit the 2D
 670 nature of heat transfer in the enclosure. As the rate of heterogeneity increases to $\sigma = 2$ and 4
 671 (Figs. 10b and 10c), the isothermal surfaces become increasingly distorted inside the
 672 enclosure. The transition zone becomes narrow close to the hot and cold boundaries near $Y=1$,
 673 and wide near $Y=0$. This is because although the three cases take the same large-scale
 674 Rayleigh number, the rising of the rate of heterogeneity leads to an increase of the local
 675 Rayleigh number near $Y=1$, and a decrease of that near $Y=0$. Basically, the higher local
 676 Rayleigh number intensifies the flow velocity and enhances the convective heat transfer in the

677 vicinity of $Y=1$. The opposite effect is found near $Y=0$. Therefore, a correlation between the
678 isothermal surfaces and the rate of heterogeneity is observed for this configuration: the higher
679 the rate of heterogeneity, the more distorted the temperature iso-surfaces. Contrarily, for the
680 H-het configuration (Figs. 10d-10f), the impact of heterogeneity is much less evident
681 influence on the shape of isothermal surfaces. The three cases exhibit a typical 3D nature of
682 heat transfer in the enclosure. Unlike the V-het configuration, the 3D effect for the H-het
683 configuration originates from the varying temperature boundary condition, rather than
684 heterogeneity. Increase of rate of heterogeneity only causes a slight change in the shape of
685 isotherms in the bottom half of the $X=0, Y=0$ edge, where the transition zone becomes wider
686 due to the decrease of local Rayleigh number that reduces the convective heat transfer at this
687 region.

688



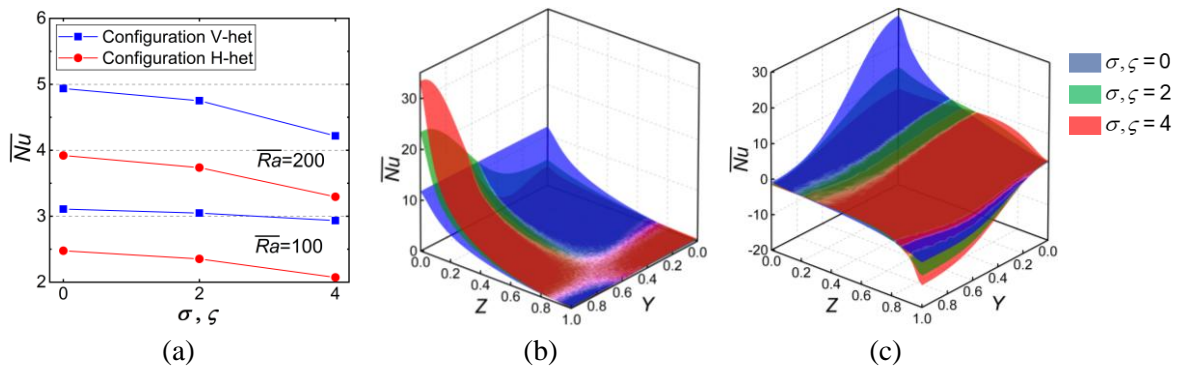
689 **Fig. 10.** Effect of heterogeneity on temperature distribution: Main temperature iso-surfaces
690 for the configuration V-het (top) and H-het (bottom) for $\overline{Ra} = 100$.

691

692 The effect of heterogeneity on the heat flux through the hot wall is shown in Fig. 11, which
693 displays the variation of the average Nusselt number (\overline{Nu}) as a function of the rate of
694 heterogeneity (σ for the V-het configuration and ζ for the H-het configuration) for two
695 different values of large-scale Rayleigh number. The results show that in both configurations,
696 the average heat flux to the domain decreases with the increase of the rate of heterogeneity.
697 The effect of rate of heterogeneity on the heat flux is more significant at high Rayleigh
698 regimes, which highlights that the reduction of heat thermal gradients in low permeability
699 zones is slightly more relevant than their increase in regions of high permeability. The
700 reduction is not large, but relevant for a proper understanding of entropy generation
701 dependence on heterogeneity.

702 The spatial variations of the local Nusselt number on the hot wall for configurations V-het and
703 H-het are depicted in Figs. 11b and 11c, respectively. For the V-het configuration, the
704 increase of the rate of heterogeneity enhances the heat flux to the domain at the high
705 permeable zone and reduces it in the low permeable zone. The opposite is true in the H-het
706 configuration, where the maximum local Nusselt number can be observed in the zone of low
707 permeability.

708



709 **Fig. 11.** Effect of heterogeneity on heat flux through the hot wall: (a) the average Nusselt
710 number, (b) and (c) maps of local Nusselt number of the hot wall for the configurations V-het
711 and H-het with $\overline{Ra} = 100$, respectively.

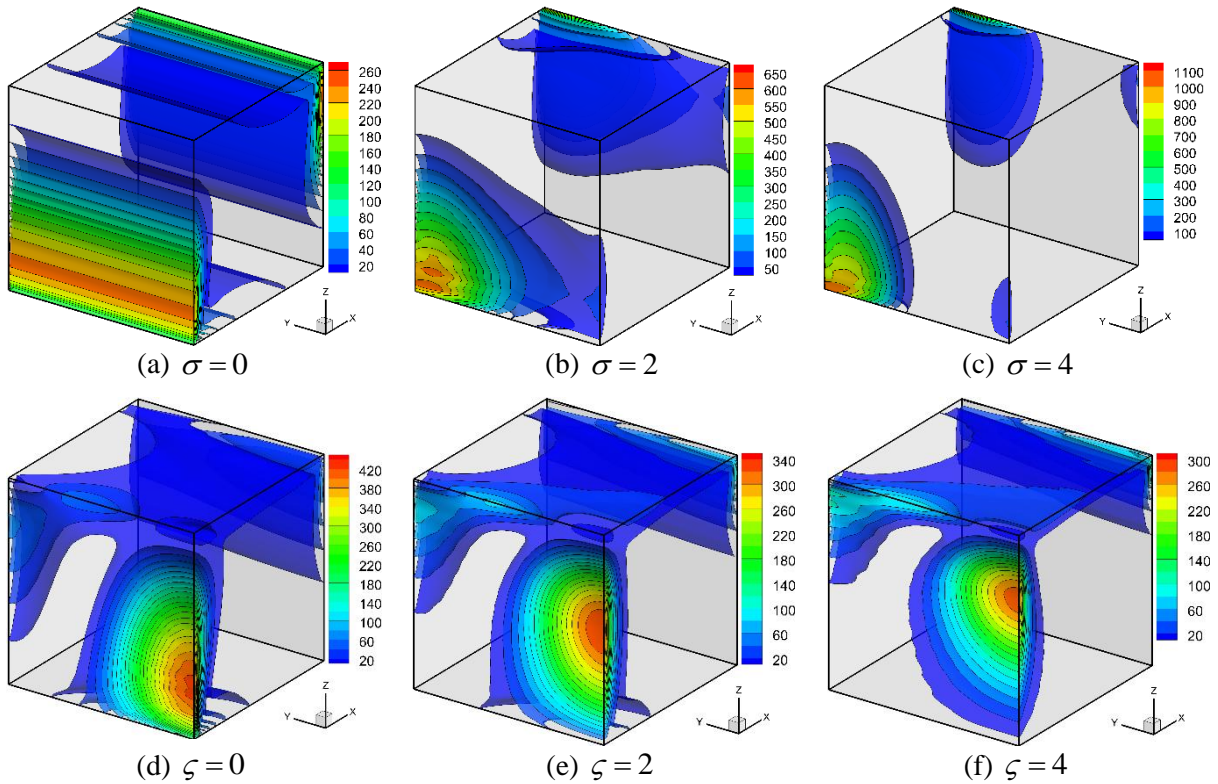
712

713 Fig. 12 depicts the local entropy generation number N_E for both configurations with varying
714 rate of heterogeneity. The 2D nature of the homogeneous ($\sigma = 0$) V-het configuration also
715 shows on the local entropy generation, which does not change along the Y axis (Fig. 12a). As
716 the rate of heterogeneity increases, the local entropy generation varies along the Y axis.
717 Specifically, the zone of maximum local entropy generation moves toward the corner in the
718 vicinity of $Y=1$, where the local Rayleigh number near $Y=1$, which intensifies both the
719 temperature gradient (Figs. 10a, b, and c) and the fluid flux (Figs. 9a, b, and c). Both increases
720 trigger an increase on the maximum local entropy generation. For the H-het configuration
721 (Figs. 12d-12f), a negative correlation between the heterogeneity rate and the maximum local
722 entropy generation is found: the higher the rate of heterogeneity, the smaller the maximum
723 value of local entropy generation (see the color scale). It should be noted that the effect of the
724 heterogeneity rate on the maximum value of local entropy generation is not very evident for
725 this configuration. This is because for the H-het configuration, neither the temperature
726 gradient nor the maximum velocity change much with the variation of heterogeneity rate (see
727 Figs. 9 and 10). In the vicinity of hot wall at $X=0$, the zone of maximum local entropy
728 generation moves upward with the increase of heterogeneity rate, which is consistent with the
729 velocity field (Fig. 9), as the higher heterogeneity rate increases the local Rayleigh number
730 near $Z=1$ and decreases that near $Z=0$, which further influences the fluid flow and modifies
731 the distribution of local entropy generation. It may be noticed, however, that the maximum
732 entropy generation occurs slightly below the maximum velocity, which reflects that thermal
733 gradients are highest in the lower part (Fig. 10) and contribute to the mixing term of entropy
734 generation.

735 Fig. 13 depicts the variation of the total entropy generation number (N_{tot}), the total mixing
736 rate (N_T), and the average Bejan number (\overline{Be}) as a function of the rate of heterogeneity.
737 The most important observation is that both total entropy generation and mixing rate are

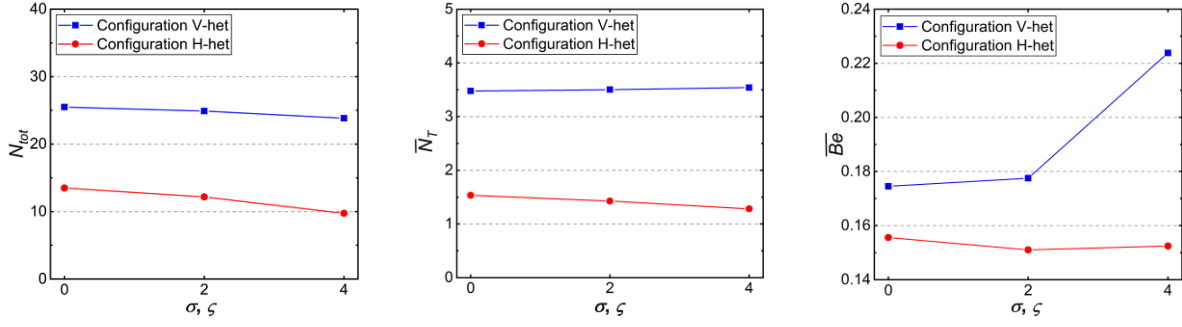
738 virtually insensitive to heterogeneity, which implies that the adopted effective permeability is
739 indeed appropriate. The total entropy generation number decreases slightly as the
740 heterogeneity level increases for both configurations, which is probably due to the shrink of
741 the active zone for local entropy generation. This phenomenon is also observed in Fig. 9,
742 where the flow velocity field shows similar profiles. N_{tot} slightly decreases with the increase
743 of the rate of heterogeneity. The average Bejan number demonstrates that the irreversibility
744 due to fluid flow has a dominant influence on the total entropy generation in the domain.
745 Similar to the total entropy generation number, in the H-het configuration, \overline{Be} decreases with
746 the increase of the rate of heterogeneity. In the opposite, for the V-het configuration, \overline{Be}
747 significantly increases with the increase of the rate of heterogeneity.

748



749 **Fig. 12.** Effect of heterogeneity on entropy generation: Iso-surfaces of local entropy
750 generation number (N_E) for the V-het configuration (top) and H-het (bottom) for $\overline{Ra} = 100$.

751



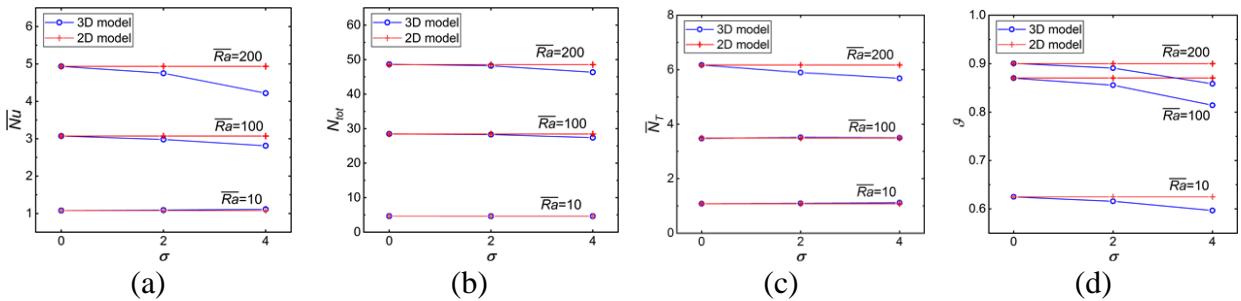
752 **Fig. 13.** Effect of heterogeneity on entropy generation: The total entropy generation number (
 753 N_{tot} , left), the total mixing rate (N_T , center), and the average Bejan number (\overline{Be} , right) for
 754 the configurations V-het and H-het ($\overline{Ra} = 100$).
 755

756 4.5 Third dimension effect

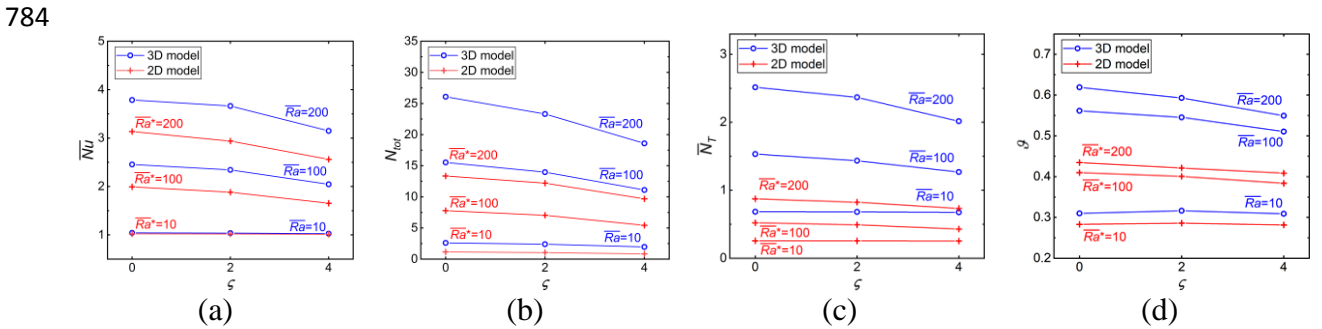
757 The goal of this section is to evaluate the effect of the third dimension on the convective flow,
 758 heat transfer, and entropy generation. Thus, we compare the 3D results with those of
 759 equivalent 2D models. For the V-het configuration, the third dimension effects are caused by
 760 heterogeneity. Hence, in the equivalent 2D model, we consider a homogenous domain with
 761 equivalent permeability as defined in the large-scale Rayleigh number (Eq. (41)). Under this
 762 assumption, the 3D model can be simplified to 2D. For the H-het configuration, the third
 763 dimension effects are related to the variable boundary conditions. Thus, in the equivalent 2D
 764 model, we keep the heterogeneity but we assume a constant temperature on the hot wall
 765 which is equal to the average temperature ($\vartheta = \int_0^1 f(Y)dY = 0.5$). For the sake of brevity, we
 766 do not consider spatial maps of temperature and entropy generation, but just compare the 2D
 767 and 3D results in terms of the average Nusselt number as metric of heat transfer, the total
 768 entropy number, and the dimensionless mixing rate (as metrics of entropy generation), and the
 769 dimensionless temperature at the top center point ($X=0.5, Y=0.5, Z=1$ for 3D cases, and $X=0.5,$
 770 $Z=1$ for 2D cases).

771 Fig 14 depicts the variation of these metrics with respect to the large-scale Rayleigh number
 772 for both 2D and 3D models with varying rates of heterogeneity for V-het configuration.

773 Obviously, 2D results insensitive to heterogeneity because the V-het 2D model is
 774 homogeneous and identical to the 3D model with $\sigma = 0$. Therefore, the 3D effect is similar to
 775 the effect of heterogeneity discussed in the previous section. Therefore, the 2D assumption
 776 leads to an overestimation of the heat losses and average Nusselt number (Fig. 14a). But the
 777 impact is small in terms of both total entropy generation and mixing rate (Figs. 14b and c).
 778 The discrepancy between 2D and 3D models is more significant at high Rayleigh regimes.
 779 As the 3D effects are caused by the heterogeneity, it is clear in Fig.14 that the increase of the
 780 rate of heterogeneity enlarges the discrepancy between 2D and 3D models.



781 **Fig. 14.** Third dimension effect on the (a) average Nusselt number, (b) total entropy
 782 generation number, (c) the dimensionless mixing rate, and (c) temperature at the top center
 783 point for the V-het configuration.



785 **Fig. 15.** Third dimension effect on the (a) average Nusselt number, (b) total entropy
 786 generation number, (c) dimensionless mixing rate, and (d) temperature at the top center point
 787 for the configuration H-het.

788
 789 The H-het configuration yields more interesting results than V-het. The 2D model largely
 790 underestimates all indicators (Fig. 15). Simplifying to 2D (i.e., neglecting temperature
 791 variability in the hot face of the enclosure) reduces somewhat the heat flux (Nusselt number,
 792 Fig. 15a) and leads to a more homogeneous flow and temperature distribution. Lack of
 793 variability leads to a dramatic reduction in total entropy generation (a factor around 2, Fig.

794 15b) and even more in mixing rate (a factor around 3, Fig. 15c). The absolute value of the
795 discrepancy between 2D and 3D simulations is more significant at high Rayleigh numbers. A
796 hint on the reason for the discrepancy can be gained from the temperature at the middle of the
797 top face (Fig. 15d). High permeability at the top causes active fluid circulation, so that
798 temperature at the top face approaches asymptotically the temperature of the hot face (0.5 in
799 the 2D case) as the Rayleigh number increases. However, circulation is most active near the
800 hot end of this face in the 3D case (recall Fig. 9). As a result, temperature at the middle of the
801 top face is above the average temperature of the hot face (Fig. 15d), which explains the large
802 increase in the mixing rate.

803

804 **5 Conclusions**

805 In this work, we investigate three-dimensional natural convection and associated entropy
806 generation in heterogeneous porous media under steady-state conditions. Two typical
807 configurations are considered: one has vertically stratified porous media and subject to
808 constant temperature boundary conditions, the other has horizontally stratified porous media
809 and subject to spatially varying temperature boundary conditions. Both configurations lead to
810 three-dimensional flow conditions that cannot be simplified to two-dimensions. The 3D effect
811 of the first configuration comes from the heterogeneity in permeability, while that of the
812 second configuration originates from the varying temperature boundary conditions. As 3D
813 simulations are computationally expensive, the Fourier series (FS) method is used to obtain
814 highly accurate solutions in affordable CPU time. The comparison between the FS and finite
815 element methods (COMSOL) confirms the validity of the new developed FS solutions, which
816 provide a highly accurate three-dimensional benchmark for testing numerical codes.

817 The solution is different for each configuration. In the V-het configuration, the typical
818 convection cell of 2D natural convection increases its vorticity and splits into two vortices as

819 heterogeneity increases. In the H-het configuration, the variable temperature of the hot face
820 causes the vortex to curve into a quarter of a torus whose axis displaces upwards as
821 heterogeneity increases. Comparison between 2D and 3D simulations shows that the 2D
822 assumption underestimates the heat flux to the domain, the entropy generation and the
823 temperature on the top surface. The underestimation is dramatic in the horizontally stratified
824 case.

825 We propose an effective large-scale Rayleigh number to characterize natural convection in
826 heterogeneous media. This new large-scale Rayleigh number is similar to the standard
827 Rayleigh number for homogeneous media, but using the arithmetic average of the
828 heterogeneous permeability. Based on the FS solutions, we investigate the effect of this
829 effective Rayleigh number and level of heterogeneity on heat and fluid flux, as quantified by
830 the Nusselt number (dimensionless heat flux) and entropy generation (both from viscous
831 dissipation and mixing). Results reveal that, as expected, the increase of the effective
832 Rayleigh number considerably intensifies the fluid flow and enhances the convective heat
833 transfer, inducing high-temperature gradients and large local entropy generation near the
834 boundaries and, thus, within the enclosure. These increases lead to a large increase of total
835 entropy generation, in terms of both viscous forces dissipation and mixing rate.

836 Perhaps more surprisingly, we find a very mild but negative correlation between the
837 heterogeneity rate and entropy generation for both configurations. In fact, both total entropy
838 and, especially, mixing rate remain virtually constant, despite a reduction of heat flux (Nusselt
839 number) when heterogeneity increases. This is important because it suggests that the proposed
840 Rayleigh number is indeed sufficient to explain the impact of heterogeneity on dissipative
841 processes and dissolution/precipitation reactions in cases where density variations are driven
842 by changes in composition, so that mixing controls reaction rates (such as in CO₂ dissolution
843 in carbon storage problems). But it is surprising for two reasons. First, for a given effective

844 permeability, one would expect both fluxes and temperature (concentration) gradients to
845 increase with heterogeneity. Second, the arithmetic average is the largest of all reasonable
846 averages (in fact, it is the effective permeability only for ideal infinite dimension geometries),
847 so that one would expect other more traditional averages (e.g., geometric or 1/3 power
848 averaging) to work better. We conclude that the explanation lies in this double paradox. Had
849 we chosen any other average for permeability and large-scale Rayleigh number, we would
850 have found that, indeed, entropy generation increases with heterogeneity when the Rayleigh
851 number is fixed. Further, as the heat (solute mass) flux drops when increasing heterogeneity
852 while fixing Rayleigh number, the expectation of increased disorder turns out to be correct for
853 a fixed boundary heat (solute mass) flux. In summary, the proposed Rayleigh number would
854 not be appropriate for predicting boundary fluxes, which might require using the traditional
855 effective permeability, but it is excellent in predicting entropy generation indicators, which
856 become virtually insensitive to heterogeneity.

857

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860 No. 11702199). The data used in this work are available on the GitHub repository:
861 <https://github.com/fahs-LHYGES>.

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