Capillarity

Vol. 9, No. 1, p. 1-8, 2023

Short communication

The impact of wettability and fluid saturations on multiphase representative elementary volume estimations of micro-porous media

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Keywords:
Permeability
asymptotic homogenization
thermodynamic bounds
pore scale modelling
REV sensitivity

Cited as:
Hussain, S. T., Regenauer-Lieb, K., Zhuravljov, A., Hussain, F., Rahman, S. S. The impact of wettability and fluid saturations on multiphase representative elementary volume estimations of micro-porous media. Capillarity, 2023, 9(1): 1-8.
https://doi.org/10.46690/capi.2023.10.01

Abstract:
The occurrence of multi-phase flows in porous media is a complex phenomenon that involves multiple scales, ranging from individual pores to larger continuum scales. Upscaling frameworks have emerged as a response to the need for addressing the disparity between micro-scale processes and macroscopic modelling. Determination of the representative elementary volume is important for understanding fluid dynamics in micro-porous materials. The size of the representative elementary volume for multiphase flow in porous media is significantly affected by wettability and fluid saturations. Previous studies have overlooked this aspect by conducting simulations under conditions of constant medium wettability and fluid saturations. This study uses finite volume simulations with a volume of fluid approach for two distinct asymptotic homogenization methods, namely hydrodynamic bounds of relative permeability and thermodynamic bounds of entropy production. Strong wetting conditions with high wetting phase saturation were found to require a smaller sample size to establish representative elementary volume, while mixed-wettability scenarios necessitate the largest sample sizes. These findings improve our understanding of multiphase fluid flow behaviour in micro-porous materials and aid in enhancing techniques for scaling up observations and predictive modelling in engineering and environmental fields.

1. Introduction

The investigation of transport phenomena in porous media holds significant importance across various disciplines, such as hydrogeology, petroleum engineering, environmental science, and materials engineering (Bear, 1973; Werth et al., 2010; Bultreys et al., 2016; Jahanbakhsh et al., 2020). Historically, experimental measurements have played a pivotal role in research within this field, providing vital insights into the dynamics of fluid flow and the solute transport. Nevertheless, the advent of image-based computations signifies a paradigm shift in the field of porous media research, presenting a multitude of persuasive justifications for prioritising computational methodologies over conventional experimental methods (Liu and Regenauer-Lieb, 2021; Shapoval et al., 2022). To begin with, it is worth noting that image-based computations provide an unparalleled level of detail and spatial resolution. Attaining such a high degree of accuracy is a formidable task when relying on experimental methods, since the capabilities of instrumentation frequently impose constraints that confine observations to more substantial magnitudes (Pirzada et al., 2018). Furthermore, the utilisation of computational

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Received August 1, 2023; revised August 16, 2023; accepted September 2, 2023; available online September 5, 2023.

Yandy Scientific Press

simulations in the field of porous media transport enables the investigation of intricate and ever-changing phenomena. Researchers are afforded the opportunity to explore a diverse array of scenarios, encompassing multiphase flow, non-Newtonian fluid behaviour, and reactive transport, with a notable degree of convenience (Alpak et al., 2018; Zhao et al., 2019; Lanetc et al., 2022). In addition, the utilisation of image-based calculations contributes to the improvement of repeatability and comparability of outcomes. The replication and collaborative use of computational models among researchers can effectively guarantee the consistency of research findings.

In the context of representative elementary volume (REV) estimation, the precise determination plays a crucial role in forecasting the overall flow characteristics and formulating effective reservoir management approaches. REV is greatly influenced by the relative permeability of fluid, which is highly dependent on pore-scale characteristics and interfacial fluid dynamics (Janetti et al., 2017; Liu and Wang, 2022). Various factors such as viscosity ratio, capillary number, medium wettability, and initial fluid saturations have been found to have an impact on the relative permeability (Hussain et al., 2021; Mahmud, 2022; Xiao et al., 2022). The comprehension of the impacts of wettability and fluid saturations on REV estimate has profound implications for a wide range of applications, including but not limited to oil recovery, CO_2 sequestration, and groundwater management (Costanza-Robinson et al., 2011; Janetti et al., 2017; Huang et al., 2021).

When estimating REV for micro-porous structures, the occurrence of multi-phase flows is a prevalent phenomenon (Porta et al., 2013; Jackson et al., 2020). Despite recent progress, our understanding of these flows remains insufficient. The current collection of literature (Mostaghimi et al., 2013; Guadagnini et al., 2014; Liu et al., 2018, 2021; Singh et al., 2020; Liu and Regenauer-Lieb, 2021) lacks the ability to effectively analyze the dynamics of multiphase flows. Instead, these studies primarily rely on geometric reasoning or simulations of single-phase flows to validate the REV assumption. In order to tackle this intricate issue, many upscaling frameworks have been devised and used to create REV models that effectively include essential characteristics seen at the pore-scale level. The upscaling models often used an effective medium approach to homogenize micro-scale characteristics and the dynamics of multiphase flow (Gray and Miller, 2014; Liu and Wang, 2022). Regenauer-Lieb et al. (2014) laid the groundwork of a robust theoretical framework for calculating the REV and evaluating uncertainty. The approach determines the smallest feasible REV size by analysing the maximum and minimum entropy generation rates caused by the interaction of hydromechanical thermodynamic forces and fluxes. Icardi et al. (2016) further emphasized the need of including uncertainty in pore-scale physics to enhance its applicability in upscaling models. Hussain et al. (2023) carried out a comprehensive analysis of uncertainty quantification in the investigation of pore-scale physics, with the objective of enhancing the accuracy and reliability of upscaling models. The authors presented hydrodynamic and thermodynamic bounds for the flow of multiple phases through sandstone and carbonate samples. Additionally, they defined REVs for a multiphase system by using Dirichlet and von Neumann boundary conditions. However, the understanding of combined influence of the unknown geometry of an elementary cell, the wettability of the medium, and the initial fluid configurations on predictions of the REV is still lacking.

The objective of this research is to examine the impact of wettability modification and variations in initial saturations on the estimate of REV in a micro-porous structure of a sand pack, specifically focusing on steady-state immiscible two-phase flows. The study employs numerical simulations that utilise the finite volume technique with OpenFoam's volume of fluid (VOF) methodology, together with customised variable mesh generation methods. VOF approach enables the incorporation of thermodynamic couplings and if the approach effectively resolves the instabilities, it is expected that the results will smoothly align with the upper and lower limits of entropy generation. This work expands upon the prior research (Hussain et al., 2023) and provide valuable insights into the optimisation of simulation parameters for REV applications. Through the examination of the impact of wettability and initial saturations on the REV, this study enhances our comprehension of multi-phase flow phenomena inside porous media and facilitates the integration of micro-scale mechanisms with macroscopic modelling approaches. Additionally, the results obtained from this work have the potential to provide valuable insights for determining the most suitable parameters for scaling up approaches and enhancing the dependability of predictive models in a range of technical and environmental contexts.

2. Methodology

Main purpose of this study is to broaden the extent of our prior investigation (Hussain et al., 2023). The fundamental workflow pertaining to image processing, pore scale modelling, and post-processing of data remains consistent in this research, except for the incorporation of new factors, namely wettability and initial fluid configurations. The VOF method utilized is an interface capture method based on saturations that was created for the modelling of two-phase incompressible flows. This VOF system of partial differential equations can only be resolved numerically while considering arbitrary scenarios. The pressure-implicit with splitting of operators, the semi-implicit approach for pressure-linked equations, or a combination of these are examples of adaptable numerical algorithms (Patankar, 2018). These methods are implemented in the OpenFoam open-source project, which is based on the finite volume technique (Moukalled et al., 2016) and has a variety of pre-validated solvers including InterFoam (Deshpande et al., 2012) as well as collections of CFD and auxiliary C++ libraries (Greenshields, 2022).

In the context of determining entropy for non-isothermal transport of multi-phase fluids in porous media, the research conducted by Kjelstrup et al. (2018) offers a comprehensive analysis and a versatile set of equations that can be applied to various fluid flow scenarios. Furthermore, the derivation of dissipative material characteristics employs an original approach that incorporates thermodynamic uncertainty quan-

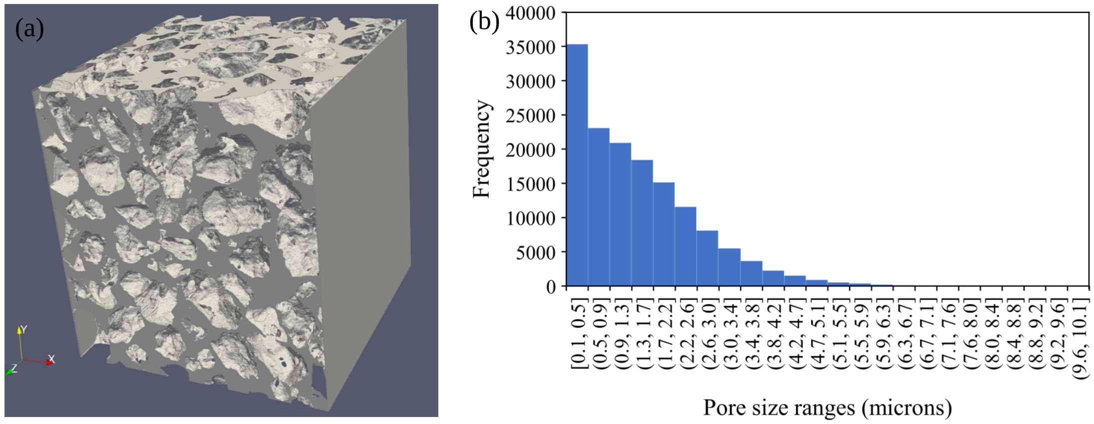

Fig. 1. Pore space representation of (a) sand pack configuration at 600^3 voxels ($3.12\ mm^3$) and (b) its pore size distribution.

tification, and it is more reliable than the conventional effective medium theory. It also implies that the REV must be larger than that predicted by the traditional methods in order to provide thermodynamic robustness. The main advantage of the applied technique is the definition of uncertainty quantification because the effective medium theory often results in a single value, but the thermodynamic approach allows for the specification of uncertainty through upper and lower bounds of the material characteristics. To get an in-depth examination of the simulation methodology, mesh generation, and post-processing computations, readers are advised to consult the authors' recent publication (Hussain et al., 2023) and the associated references.

In addition, the geometrical expansion method has been modified to accommodate multiphase conditions due to the absence of observations about the impact of saturation changes in previously used volume increments. Hence, a greater amount of computing resources was necessary for each rock configuration in order to document the aims of this research.

2.1 Data acquisition and image processing

The segmented data of a sand pack was obtained from Singh et al. (2020) and can be accessed online via the digital rocks portal. Sand pack was chosen as the subject of investigation due to the primary aim of assessing the sensitivity of the REV to variations in wettability and saturations, regardless of the specific rock type. Hence, the use of a heterogeneous rock will inevitably result in an increase of both computational expenses and time requirements. The homogeneity of the sand pack is clearly demonstrated by the pore size distribution depicted in Fig. 1(b), which shows abundant occurrences of multiple pore size ranges. The micro-CT scans were performed at the Tyree X-ray micro-CT facility located at the University of New South Wales in Sydney, Australia. The segmentation process was conducted using the watershed technique in Avizo™ software. Subsequently, the images were cropped using custom Python™ algorithms that relied on the NumPy library. These algorithms enabled isotropic increments in the domain size, with each increment consisting of 25^3 voxels. This process was repeated until the desired REV sizes were attained. Flow simulations and image processing were conducted using the AMD Ryzen™ 5950X processor, which was complemented by the NVIDIA GeForce RTX 3080 graphics processing unit and a substantial 128 GB of random-access memory.

2.2 Discretization and grid convergence

The SnappyHexMesh tool from OpenFoam was used for the purpose of discretizing micro-CT images in order to facilitate simulations (Greenshields, 2022). The use of this particular tool facilitates the generation of rudimentary initial meshes as well as two-dimensional and three-dimensional hexahedral meshes derived from triangulated surface geometry. The meshes undergo many iterative procedures in order to enhance and transform them, ultimately resulting in the triangulated surface geometry. A supplementary Python™ script was developed to extract a triangulated surface geometry from a segmented micro-CT image, in order to perform the aforementioned meshing approach. Additionally, the Python™ script has the capability to construct additional layers for the inlet and outflow boundaries, produce the associated initial mesh, and assemble the outcomes into an OpenFoam case by using the suitable templates and supplementary parameters.

The resolution of the mesh significantly impacts the results of flow simulations, leading to discrepancies in the outcomes. Hence, the attainment of grid convergence becomes necessary in order to ascertain the most suitable mesh dimensions for a given rock sample. In the present sand pack configuration, it was observed that using a mesh enlargement criterion of 7 yielded results that were equal to those obtained using a more refined mesh enlargement criterion of 4.

2.3 Benchmarking

The objective of this study is to exclusively examine the impacts of wettability and fluid saturations on REV estimations. To do this, a basic rock configuration was selected from the research conducted by Singh et al. (2020). Upon conducting a thorough literature study, it was discovered that the aforementioned research paper stands as the sole publication that provide REV calculations specifically for current sand pack structure. Hence, it is advisable to compare our findings with those of previous studies; although, it is worth noting that the latter did not consider the influence of multiphase flows. Based on our comprehension, the effective benchmarking of our model with their results for the sand pack demonstrates a substantial concurrence between the two, hence serving as a validation of our findings. Fig. 2 displays the normalised values of porosity and permeability obtained from Singh et al. (2020)'s study, as well as the normalised values generated by our model, where normalisation is based on the largest sample in the dataset. There is a strong agreement observed in the results generated by both methodologies.

3. Results and discussions

3.1 Single-phase configuration

The absolute permeability and entopic bounds were determined by the use of a three-dimensional model that was obtained from micro-CT image of sand pack (see Fig. 1(a)). Numerical simulations were conducted using pressure constant (PC) and velocity constant (VC) boundary conditions. Fig. 3(a) illustrates the results of single-phase REV measurements, illustrating the upper and lower bounds of stabilized absolute permeabilities. The data indicates that as the sample size increases, the absolute permeability for both PC and VC approaches a common value that is within the range of uncertainty, which vary from 2.4 to 7.6 Darcy. This can be noted in Fig. 3(a), which illustrates the absolute permeability bounds for PC and VC, as well as in Fig. 3(b), which depicts the entropic bounds for PC and VC. The documentation of the validity of a continuum assumption is achieved via the use of two asymptotic homogenization methodologies. The hydrodynamic REV has reached convergence for sand pack configuration with sizes over 150 cubic voxels, whilst the thermodynamic REV is established for sizes beyond 200 cubic voxels, approximately equivalent to 0.78 and 1.04 mm^3, respectively.

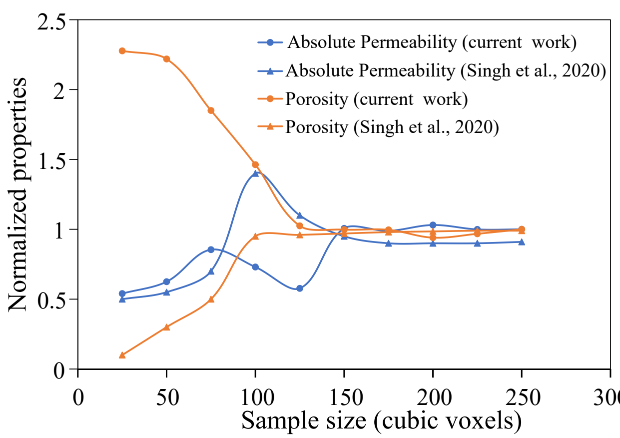

Fig. 2. Model benchmarking for sand pack with data produced by Singh et al. (2020).

3.2 Multi-phase configuration

This section provides an analysis and interpretation of the findings pertaining to the central focus of this publication, namely the influence of wettability, initial fluid configurations, and pore scale characteristics on the estimation of REV through the utilisation of relative permeability (K_r). Previous study (Hussain et al., 2023) showed that the flow rate of the PC boundary condition exhibits variations throughout the sample as a result of uncontrolled capillary numbers. Consequently, the estimation of the multiphase REV in this study is solely based on the utilization of the VC boundary condition for the estimations of K_r values.

3.2.1 Hydrodynamic bounds

Fig. 4 illustrates the multiphase REV estimations of the sand pack configuration, taking into account the asymptotic homogeneity of VC hydrodynamic bounds. The wetting phase relative permeability exhibits an increasing pattern as the wetting phase saturation rises across all scenarios, whereas the non-wetting phase relative permeability shows a decline (refer to Fig. 4). The reason for this phenomenon is the variability in the initial wetting conditions, which leads to

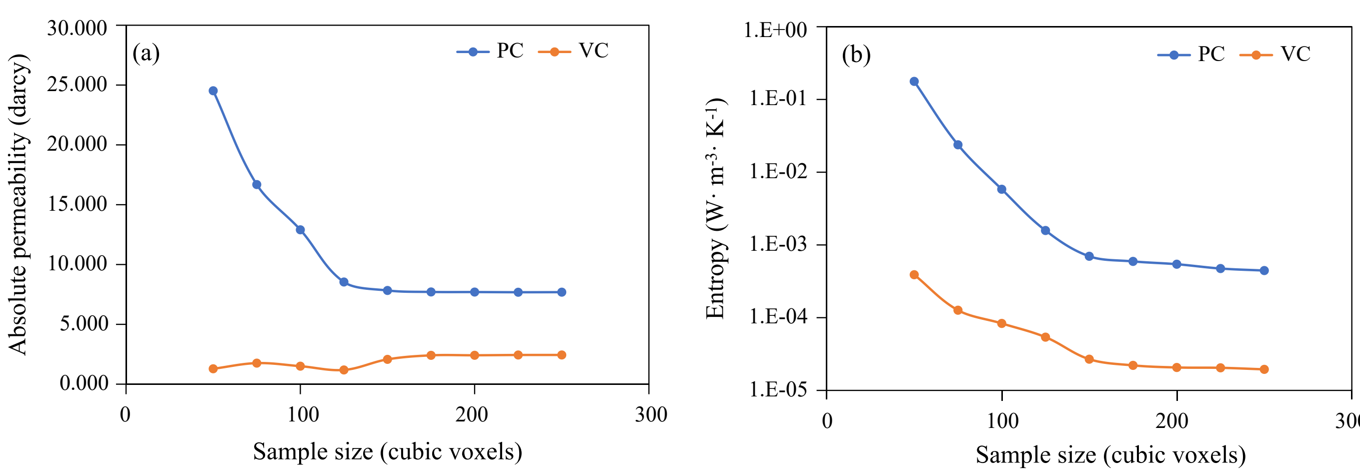

Fig. 3. Asymptotic homogenization of upper and lower (a) hydrodynamic bounds for absolute permeabilities and (b) thermodynamic bounds for entropy production.

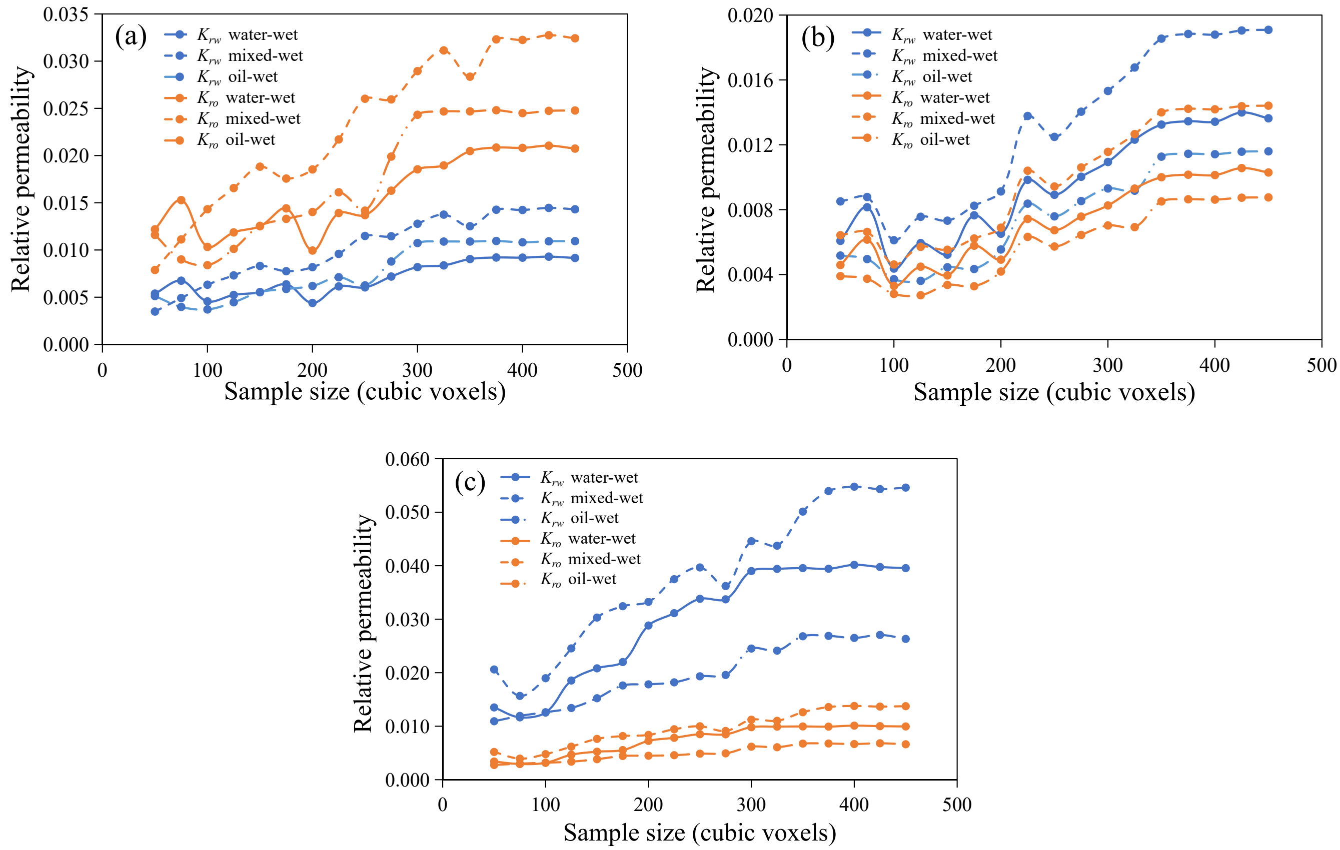

Fig. 4. Constant flux hydrodynamic bounds for relative permeabilities of oil and water at (a) 25% water and 75% oil saturations, (b) 50% water and 50% oil saturations and (c) 75% water and 25% oil saturations.

a higher oil relative permeability (K_{ro}) compared to water relative permeability (K_{rw}) at lower water saturation (S_w) levels (refer to Fig. 4(a)). As the water saturation rises, the system exhibits enhanced mobility for the water phase (refer to Fig. 4(c)). The observed behaviours align with the usual relative permeability curves often seen in oil-wet and water-wet systems. Significant variations in REVs are observed due to changes in wettability and the initial configurations of fluids. The aforementioned observations have been consolidated and presented in Table 1. According to the data gathered, it is evident that the establishment of REVs requires a minimum volume of 300 cubic voxels (equivalent to 1.56 mm^3). This criterion is applicable to systems characterized by a significant presence of wetting phase saturations and strong wetting conditions. For instance, in scenarios where the system is oil-wet with a phase saturation of 25% S_w or water-wet with a phase saturation of 75% S_w. In contrast, systems with opposing characteristics, such as water-wet scenarios with a saturation of 25% S_w and oil-wet scenarios with a saturation of 75% S_w, exhibit REVs that exceed 350 cubic voxels (equivalent to 1.82 mm^3). Additionally, it should be noted that systems with higher relative permeability values need larger samples to establish REVs. For instance, in mixed-wet situations with water saturations of 25% and 75%, the required volume exceeds 375 cubic voxels (equivalent to 1.95 mm^3). With regards to systems with a saturation of 50% S_w (refer to Fig. 4(b)), all scenarios demonstrate REVs above 350 cubic voxels (equivalent to 1.82 mm^3). This inability to demonstrate the impacts of fluid configurations on REV calculations was observed in earlier research (Hussain et al., 2023). Moreover, the data also suggest that the multiphase REV with various wetting scenarios exceeds the single-phase estimate by a factor of more than two in the case of a homogeneous rock arrangement, such as a sand pack.

Table 1. Sensitivity of hydrodynamic REV (in cubic voxels) with wettability and initial fluid saturations.

Wettability	Initial water saturations		
	25%	50%	75%
Water-wet (45°)	350	350	300
Mixed-wet (90°)	375	350	375
Oil-wet (135°)	300	350	350

3.2.2 Thermodynamic bounds

Fig. 5 demonstrates an important difference in the VC bounds of the rock configuration, indicating that systems with higher relative permeability values exhibit lower stabilized entropy production compared to their counterparts. This is par-

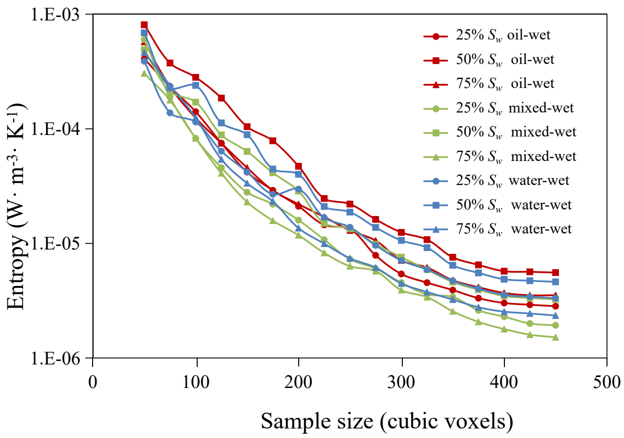

Fig. 5. Constant flux thermodynamic bounds for entropy production of all scenarios.

Table 2. Entropy production at REVs of all scenarios.

Wettability	Water saturations (%)	Stabilized entropy ($W \cdot m^{-3} \cdot K^{-1}$)
	25	3.42×10^{-6}
Water-wet (45°)	50	4.72×10^{-6}
	75	2.44×10^{-6}
	25	2.00×10^{-6}
Mixed-wet (90°)	50	3.63×10^{-6}
	75	1.59×10^{-6}
	25	2.91×10^{-6}
Oil-wet (135°)	50	5.64×10^{-6}
	75	3.52×10^{-6}

ticularly evident in mixed-wet situations at 25% and 75% S_w. Systems with 50% S_w exhibit the highest value of stabilized entropies, whereas the other systems, such as those with 25% and 75% S_w oil/water-wet scenarios, occupy intermediate positions between the two extremes. The stabilized entropy values have been compiled and shown in Table 2. As a result of these fluctuations in entropic values, the estimations of multiphase REV vary from those of single-phase systems.

In the case of single-phase scenarios, the establishment of entropic bounds has shown that REV for sand pack should consist of at least 200 cubic voxels, equivalent to 1.04 mm^3. However, in the context of multiphase scenarios, it has been deemed necessary to extend the REV sample sizes to 375 cubic voxels or more, as summarized in Table 3. The thermodynamic REVs exhibit similar tendencies to those of multiphase hydrodynamic REVs but necessitating larger sizes. Hence, the ultimate multiphase REV estimations for the present rock configuration are determined based on thermodynamic bounds, particularly those derived from the 25% and 75% S_w situations for mixed-wet scenarios. This is due to the fact that these cases need greater volumes in order to establish reliable REV values.

Table 3. Sensitivity of thermodynamic REV (in cubic voxels) with wettability and initial fluid saturations.

Wettability	Initial water saturations		
	25%	50%	75%
Water-wet (45°)	400	400	375
Mixed-wet (90°)	425	400	425
Oil-wet (135°)	375	400	400

4. Conclusions

This work investigates the influence of wettability and initial fluid saturations on the estimate of REV for multiphase flow in a micro-porous sand pack configuration. It builds upon our previous research on REV estimations for multiphase flow in sandstone and carbonate samples (Hussain et al., 2023). The pilot research did not capture these impacts due to the simulations being done under a constant wettability condition of the medium (water-wet). Additionally, the reported results did not include the effects of initial fluid saturations, perhaps because the size increments used to attain REV were too large. Hence, the current investigation represents a significant advancement in the optimization of REV estimates. It highlights the need for researchers to consider these often-ignored characteristics during the execution of such investigations. In short, this study has led to the following conclusions:

1) As the saturation of the wetting phase rises, the K_r of the wetting phase also increases, while the K_r of the non-wetting phase drops. Consequently, in instances when water-wet conditions are present and there is a high initial water saturation, the establishment of the REV will occur at an early stage. Conversely, when the initial water saturation is low, the establishment of the REV would be delayed. In the context of mixed-wet instances, when the fluids saturations of 50% are utilized, the resulting output is similar.
2) The cases that exhibit higher K_r values in each phase need larger sample sizes for establishing REVs. These cases are associated with mixed-wettability setups, namely those with 25% and 75% S_w. This phenomenon may also be seen in the REVs determined by thermodynamic approach.
3) The establishment of the final REV is determined by the thermodynamic bounds for entropy production. This is because thermodynamic stabilization requires a larger sample size than hydrodynamic stabilization, resulting in more accurate REV estimations.

To summarize, the suggested criteria for estimating the REV in multiphase systems of micro-porous media are as follows: (a) Using a medium that exhibits mixed wettability, (b) ensuring a high initial saturation of one phase, and (c) injecting both phases at an equal rate while maintaining a capillary number below 10^{-5}. This approach enables the establishment of REV to occur at the largest feasible sample size, hence yielding a more precise estimation of REV.

Acknowledgements

Shaheryar T. Hussain would like to acknowledge the support from Australian Government and University of New South Wales for providing RTP scholarship of his PhD.

Conflict of interest

The authors declare no competing interest.

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