Int. J. Renew. Energy Dev. 2025, 14 (4), 668-693

Contents list available at IJRED website

International Journal of Renewable Energy Development

Journal homepage: https://ijred.undip.ac.id

Research Article

A scoping review of numerical modelling studies of geothermal reservoirs: Trends and opportunities post-COP25

Ella María Llanos [a] and Daniela Blessent [b*]

[a]ETICA Consulting & Research, Melbourne, Australia

[b]Faculty of Engineering, Universidad de Medellín, Medellín, Colombia

Abstract. At the 28th Conference of Parties (COP28) a commitment to triple renewable energy capacity by 2030 was made. Currently at 16 GW, geothermal accounts for 0.5% of world-wide installed renewable electricity capacity. In this scoping review, Elsevier's database was used to determine the role reservoir simulation has played and could continue to play in assisting the geothermal industry in achieving COP28's goal. The review includes journal papers published in English from 2020 to 2023. Particular attention was paid to the applications of TOUGH2 and COMSOL, the benefits of Machine Learning (ML) and recent projects that could assist in promoting the geothermal industry. The topics' categories comprised: Enhanced Geothermal Systems (EGS), hydrothermal, laboratory, and technology synergies. Outcomes of a bibliometric analysis elucidate these trends: ML is vital to ensuring the optimisation of geothermal resources; EGS and cross-industry projects are showing growing global interest. The likelihood of meeting the COP28 target for geothermal would be enhanced with increased participation from the South American and African countries. However, the industry's growth in these continents is restricted by high initial investment costs, technical complexities, unclear regulatory frameworks, social acceptance, and difficulties with electrical grid integration. Suggestions for overcoming these barriers to development are proposed. A brief country case study is also presented. It focuses on the economic, environmental and technical context to understand the unique challenges and opportunities for geothermal. Finally, five areas for research and development opportunities were identified: Thermo-Hydro-Mechanical-Chemical processes, reinjection and induced seismicity, reservoir characterization, cross-industry collaborations, and laboratory studies.

Keywords: Geothermal, energy, modelling, TOUGH2, COMSOL, Machine Learning

Received: 24th Jan 2025; Revised: 29th March 2025; Accepted: 8th May 2025; Available online: 17th May 2025

1. Introduction

There has been a long history of simulating reservoirs in the petroleum industry, commencing in the late 1940s. The first simulators appeared in the mid-1950s as a product of research on numerical analysis and the development of methods for using available computers (Mattax and Dalton, 1990). Whiting and Ramey (1969) were the first to apply petroleum reservoir engineering to geothermal. They created a lumped-parameter model for the Wairakei field (New Zealand) that accounted for steam-water flow. Harlow and Pracht (1972) endeavoured to demonstrate geothermal energy extraction from Hot Dry Rocks (HDR) through the use of a single phase coupled rock-fracture model. Cheng and Takahashi (1973) and Mercer (1973) created two-dimensional models of the Hawaii and Wairakei geothermal projects, respectively. Toronyi (1974) built a two-dimensional model coupled with the wellbore and allowed only two-phase flow. Brigham and Morrow (1977) allowed some spatial variation by developing three lumped-parameter models.

Since then, more than four dozen simulators have been developed (see Table 1). These codes are often used to simulate subsurface fluid flow and heat transfer via the implementation of different numerical algorithms or methods (e.g. finite difference/element/volume; boundary/discrete element). Commercially available software packages have also been applied to geothermal modelling. There are also graphical user interfaces for some of the codes listed in Table 1. For example: Leapfrog, MView, ParaView, PetraSim, REstudio and SKUA-GOCAD(https://www.itascainternational.com/learning/tutorials/working-with-paraview-2; https://tough.lbl.gov/pre-and-post-processors/).

O´Sullivan *et al.* (2000) stated that the effective starting point for the acceptance of numerical modelling by the geothermal industry was the 1980 Code Comparison Study which tested several geothermal simulators on a suite of six problems (Stanford Geothermal Program, 1980). As geothermal reservoir simulation has evolved as a discipline, several reviews have been undertaken, all from different perspectives.

Castanier and Sanyal (1980) classified the different modelling approaches as empirical, analytical, semi-analytical and numerical. O´Sullivan *et al.* (2000) recognized advancements in the inclusion of dissolved salts or non-condensable gases and the usefulness of tracer data in the calibration step, topics that were identified as a challenge by O´Sullivan (1985). Tonkin *et al.* (2021) emphasised the need for more transient geothermal wellbore simulators. Xu *et al.* (2021) reported on improvements in discrete fracture network modelling techniques conditioned to seismic point clouds in

* Corresponding author
Email: dblessent@udemedellin.edu.co (D.Blessent)

https://doi.org/10.61435/ijred.2025.61071
ISSN: 2252-4940/© 2025.The Author(s). Published by CBIORE

Table 1
Year of release of main simulators used for geothermal reservoir modelling.

Year - Name of simulator (Reference)
1979 - SHAFT78 a predecessor of MULKOM (Pruess and Schroeder, 1980)
1981 - FEFLOW (https://www.mikepoweredbydhi.com/news)
1983 - ANSYS Fluent (https://www.nafems.org/blog/posts/analysis-origins-fluent/)
1983 - AQUA (https://www.environmental-expert.com/software/aqua3d-426833)
1983 - MULKOM - later TOUGH2 (1987) (Pruess, 1988 and https://tough.lbl.gov/tough-history/)
1983 - STARS (https://www.cmgl.ca/about)
1984 - MODFLOW (McDonald and Harbaugh, 1984)
1984 - SUTRA (Voss, 1984)
1984 - UDEC (https://www.itascacg.com/about/history)
1986 - FLAC (https://www.itascacg.com/about/history)
1987 - HST3D (Kipp, 1987)
1988 - FEHM (Zyvoloski et al., 1988)
1989 - FRACAS (Cacas, 1989)
1991 - SING (Nakanishi et al., 1995)
1991 - TETRAD - (Vinsome, 1991)
1993 - NUFT (Nitao, 1993)
1994 - HYDROTHERM (https://volcanoes.usgs.gov/software/hydrotherm/history.html)
1994 - PFC (https://www.itasca.com.au/software/pfc)
1995 - FRACTure (Kohl and Hopkirk, 1995)
1995 - GEOCRACK2D (Swenson et al., 1995)
1995 - GEOFRAC (https://erlweb.mit.edu/geofrac-and-its-applications)
1995 - GEOTH3D (Yamamoto et al., 1995)
1995 - NIGHTS (Pritchett, 1995a)
1995 - STAR (Pritchett, 1995b)
1995 - STOMP (White and Oostrom, 1995)
1996 - GMS (Owens and Holland, 1996)
1996 - FRACSIM (http://www.rift.mech.tohoku.ac.jp/en/laboratory/hashida_sato_lab.html)
2002 - AD-GPRS (Automatic Differentiation General Purpose Research Sim.) (Cao, 2002)
2003 - GMRS (https://uspto.report/TM/78901513)
2003 - SHEMAT (Clauser, 2003)
2004 - COMSOL (https://www.comsol.com/release-history)
2004 - OpenFOAM (https://openfoam.org/download/history/)
2005 - HEX-S (Kohl and Mégel, 2005)
2007 - DUMU^X (Flemisch et al., 2007; https://dumux.org/about/)
2007 - PFLOTRAN (Mills et al., 2007)
2008 - FracaFlow (https://www.beicip.com/fracaflow)
2008 - MULTIFLUX (Danko, 2008)
2008 - SPFRAC (Pritchett, 2008)
2009 - OPM (Rasmussen et al., 2021)
2009 - PANDAS (Xing et al., 2009)
2011 - FALCON (Podgorney et al., 2011)
2012 - OpenGeoSys (Kolditz et al., 2012)
2013 - CFRAC (McClure and Horne, 2013)
2013 - GEOPHIRES (Beckers et al., 2013) - Geot Techno-economic Sim. Tool
2013 - GEOS (https://www.osti.gov/servlets/purl/1248286/)
2013 - HeatEX (https://www.osti.gov/servlets/purl/1178043)
2013 - HFR-Sim (Karvounis, 2013)
2015 - MRST-AD (Krogstad et al., 2015)
2015 - OOMPFS (Franz, 2015)
2017 - ECLIPSE Geothermal (Stacey and Williams, 2017)
2019 - DARTS (Wang et al., 2019)
2019 - Volsung (Clearwater and Franz, 2019) and (Franz et al., 2019)
2020 - POREPY (Keilegavlen et al., 2021)
2020 - Waiwera (Croucher et al., 2020)

Enhanced Geothermal Systems (EGS). Gao *et al.* (2022) pinpointed the importance of refining the porosity model for accurately calculating the heat transfer process of geothermal reservoirs.

Coupling of reservoir dynamics, stresses, and fluid and heat flow processes is essential in the modelling of EGS. Combinations of thermal, mechanical, hydraulic and chemical effects by different codes for the modelling of HDR and Hot Wet Rock reservoirs were discussed by Hayashi *et al.* (1999). Similarly, Pandey *et al.* (2018) surveyed the capability of several simulators to handle coupled geothermal processes. In their multi-field coupling study, Li *et al.* (2022) highlighted the challenge of accurately characterising real fracture networks.

Sanyal *et al.* (2000) discussed the suitability of GEOCRACK, FRACTure, GEOTH3D and FRACSIM-3D for the different stages of the modelling of HDR projects. Along with STAR and TETRAD, O´Sullivan *et al.* (2001) identified TOUGH2 (Pruess *et al.*, 1999) as the most frequently used software worldwide for the modelling of hydrothermal reservoirs from 1990 to 2001. Burnell *et al.* (2012) supported the trend at that time of interfacing TOUGH2 with other software, and the flexibility offered by the open-source library of subroutines. They pointed at the lack of equations of state that could handle mixtures of water, air and carbon dioxide (CO_2) for modelling gassy geothermal fields. Progress on this front was achieved through development of advanced tools in New Zealand that support TOUGH2 such as: Leapfrog, a software that can generate a conceptual model integrating geoscientific data; TIM, a novel open-source graphical tool; Waiwera, the first open-source simulator; and a Python scripting library (Nugraha *et al.*, 2022).

A review of Machine Learning (ML) papers across all disciplines by Pugliese *et al.* (2021) included published documents from 1990 to 2020. Their study showed that between 1990 and 1998, ML publication was fairly flat, with the main fields of application being logistics and medical diagnostics. However, from the early 21st century, the number of published ML research works increased exponentially, with a peak achieved in 2016, followed by a 1-year lull, and exceptional growth observed from 2018. By 2020, 11% of ML publications were related to engineering. This shows the significance of ML to the broader engineering field. Artificial intelligence (AI) as a proxy of traditional numerical reservoir modelling, has been mostly applied to the areas of reservoir characterization, reservoir engineering, and exploration. AI has been less used in drilling, which is the high-risk phase of a geothermal project (Aljubran *et al.*, 2022). The literature review conducted by Okoroafor *et al.* (2022) showed that between 2002 and 2021, ML techniques have been applied to subsurface geothermal resource development, with an exponential increase since 2018. This aligns with the findings of Pugliese *et al.* (2021).

These collective achievements have strengthened the understanding of the behaviour of geothermal reservoirs. In turn, this has facilitated the development of geothermal as a renewable source of energy. These efforts are crucial to mitigate the impact of climate change, as stated since the first Conference of the Parties (COP) meeting in Berlin (Germany) in 1995. A main outcome from COP26 was the signing of the Glasgow Climate Pact, a call for a phase-down of coal power and a roll back of fossil fuel subsidies. Then, at COP27 (Egypt, 2022), it was stated that the energy transition, based on renewable and efficient solutions, must be equitably accelerated, and enhanced around the world.

At COP28 (United Arab Emirates, 2023) a commitment to triple renewable energy production and double its efficiency by 2030 was made. To achieve this, solar and wind will play a crucial role, but other technologies also have a part to play. Currently, geothermal accounts for a mere 0.5% of the total installed global renewable electricity capacity, reaching 16 GW by the end of 2022, (IRENA and IGA, 2023). There is also about 173 GW of installed geothermal heating capacity (Cariaga, 2023). According to the International Geothermal Association (IGA) the geothermal sector needs to triple these capacities to 48 GWe for the power sector and 520 GWt for the heating and cooling sector (Cariaga, 2023).

Gutiérrez-Negrín (2024) recently released a country-update of geothermal power for the 2020-2023 period. This comprehensive global review was based on reports of the operational geothermal plants presented at the last two World Geothermal Congresses and IGA guidelines. In the concluding remarks he mentioned that to triple the current share of geothermal electric generation worldwide, it will be necessary to develop all identified hydrothermal and unconventional resources.

It is therefore pertinent and timely to present an analysis of the state of play in the geothermal reservoir modelling area in order to support its use as a means to decarbonise global energy use. Journal papers published in English in the period 2020-2023 and indexed in the Scopus database were selected as a basis for the review. By definition, scoping reviews do not describe research findings in detail but aim to provide a means of mapping fields of study. This exercise is also useful for depicting research patterns that might affect the geothermal industry and pilot projects that deploy new or developing technologies.

The work presented here consists of an integrated examination and interpretation of the intersection of three elements, i.e. geothermal numerical modelling, ML global trends and the installed geothermal electricity capacity. Under the constraints of our search, we have identified the need to assess where and how the development of the geothermal industry could be accelerated through the use of reservoir numerical modelling and the increased use of ML applications. This work takes into account recent global projects and how geothermal is synergistically expanding into cross-industries. Given the rising interest in renewables across different disciplines, a bibliometric analysis is also provided.

In summary, it has been almost five decades since the release of the first geothermal reservoir simulator. In 2023 an outcome of the COP28 meeting was a global commitment to triple renewable energy by 2030. The beginning of this decennium has been used as the starting point for this scoping review and was chosen for two reasons. Firstly, for the rapid increase in publications referencing ML in this arena since 2018, and secondly, for the impetus provided by the COP meetings which allow only five years to demonstrate steep emissions reductions. The overall aim of the work presented here is not intended to compare software capabilities but to identify ways to accelerate the benefits of numerical modelling of geothermal reservoirs.

2. Method

The methodological framework proposed by Arksey and O'Malley (2005), as applied by Bento *et al.* (2021) in the oil and gas industry, was used as a guide for this scoping review. Four stages were followed as detailed in the following subsections.

2.1. Identifying the research question

The work presented here was motivated by the interest in identifying trends and opportunities that could assist in finding an answer to the review's research question: "*What role does reservoir simulation play in assisting the geothermal industry in achieving its goal of tripling its output by 2030?*". This main question was addressed by analysing the findings into the following groups:

- Published works after COP25
- The most frequently used simulators
- The role of Machine Learning

Derived from scanning the papers included here a guide of journals to read and publish geothermal reservoir simulation findings is provided.

2.2. Identifying relevant studies

To answer the main research question the literature search was conducted using Elsevier's Scopus. The curated selection presented in this manuscript was narrowed down through the use of the Boolean search term "AND". The search was constrained to journal manuscripts published in English between 2020 and 2023.

Following Mongeon and Paul-Hus (2015), Scopus was selected given its extensive coverage of the disciplines of geosciences and engineering. The validation (i.e. checking that the information is indeed acceptable) of the data sources and the reliability of this database is essential. Launched by Elsevier in 2004, it now has more than 90 million items and offers comprehensive author and institution profiles from advanced algorithms and manual curation. Scopus' trustworthiness has prompted its use as a bibliometric data source for large-scale analyses in research assessments, landscape studies, science policy evaluations, and university rankings (Baas *et al.*, 2020). To ensure that literature is scholarly, Scopus indexes only peer-reviewed journals which provides a solid foundation for a research work.

With regards to the Boolean searches used, the first included three terms: “geothermal” AND “software name” AND “reservoir”. The word "modelling" was not used in the initial search since it is implicit in the software´s purpose. Two factors drove the structure of the search terms. Firstly, the range of applications of most simulators listed in Table 1 include the modelling of energy production from hydrocarbon reservoirs, CO_2 storage, underground hydrogen storage, environmental remediation problems, nuclear waste disposal, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, mechanical and geochemical processes in permeable media. Secondly, the word reservoir was chosen to focus solely on the hot and permeable section of a field that can be economically exploited for geothermal energy production. Therefore, the operator AND was decided on to guarantee both terms (geothermal and reservoir) associated with each simulator were included in the resulting records. Next, a search using the terms "Geothermal" AND "Machine Learning" AND "Reservoir" was undertaken. However, since "machine learning” is not a software, the term "modelling" was added to ensure ML applications were limited to reservoir modelling. Each of the Boolean syntax searched the abstract, title and keywords for the relevant terms. Although conference proceedings and extended journal articles are both valuable for scientific purposes, the latter are deemed to be a more complete and mature representation of the research output. Additionally, proceedings are often later adapted for publications in a journal. Therefore, only peer-reviewed manuscripts were included.

Different parties are actively working towards the global call to accelerate the implementation of low emissions technologies. Progress is frequently documented and shared in any language, in the form of reports, conference abstracts, social media, among others. However, English is the lingua franca in science.

In addition to the information provided towards the end of Section 1 (Introduction), the chosen timeframe for this study acknowledges the impact of COVID-19 on the global carbon emissions reduction and any progress based on decisions taken at COP25 in December 2019. Here it was stated that a six-fold increase in renewable energy deployment would be required compared to the levels at that time, to decarbonise by 2050 the energy sector, which was responsible for two-thirds of global emissions (Marrakech Partnership for Global Climate Action, 2019). On the other hand, during the pandemic, global confinement resulted in a reduction of carbon emissions by almost 9% in the first half of 2020 (Siddique *et al.*, 2021). Hoang *et al.* (2021) stated that post-pandemic, governments faced reducing renewables or expanding investment and production tax credits to get back to where they were and keep pace with the development of clean energy projects, including geothermal.

During the scanning of the papers some publications were identified as worthy of consideration, including some in Spanish. To balance the comprehensiveness of the results presented in Section 3 (Findings), Sections 4.5 and 4.6 discuss research and development opportunities and strengths and limitations of this study, respectively.

2.3. Study selection and exclusion criterion

Step one in selecting the papers for this review consisted of using the Boolean search described in Section 2.2. The initial search for each software listed in Table 1 identified 518 publications since 1979, the year SHAFT78 was released. Four early papers were found, however source information was not available for two of them, i.e. with no available online link to the documents. The historical data showed TOUGH2, COMSOL and STARS as the three simulators most reported in the

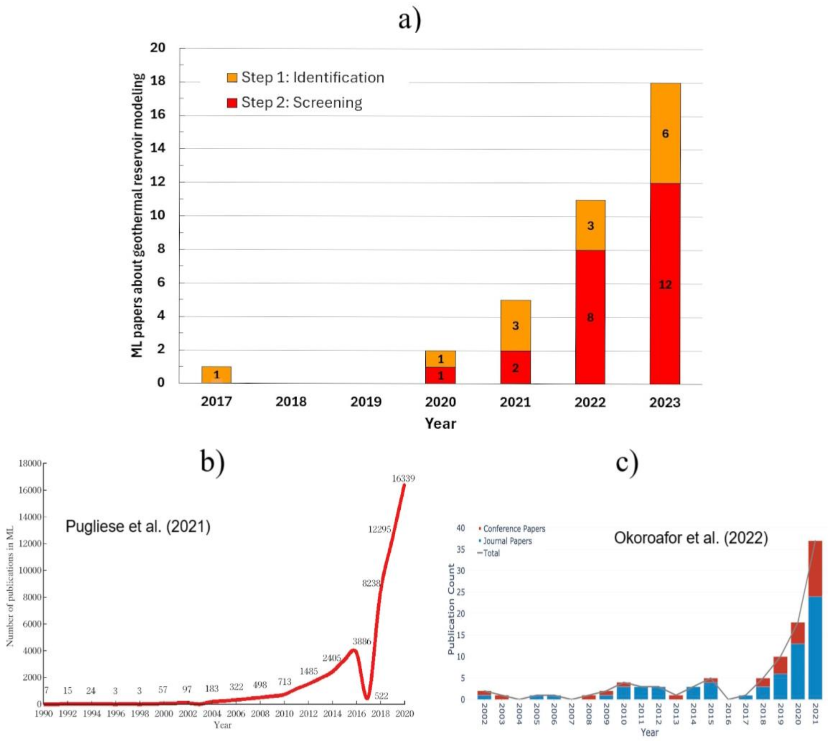

Fig. 1. ML related papers: a) Identification and screening steps in current study; b)* Pugliese et al. (2021); c)* Okoroafor et al. (2022) * with permission of the authors.

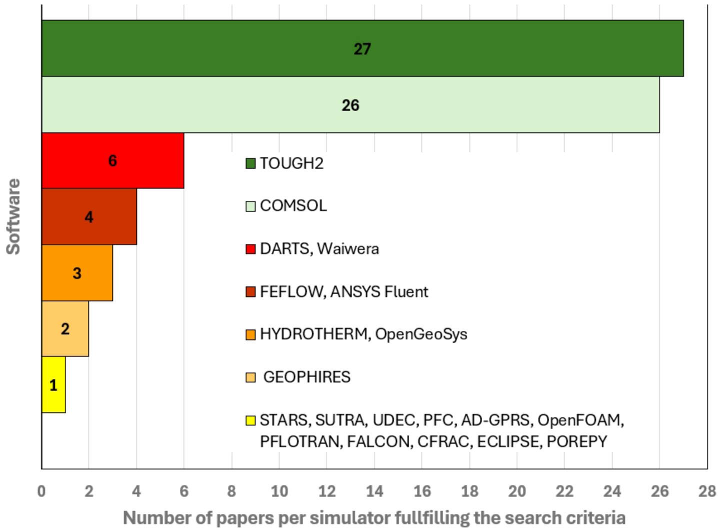

Fig. 2. Number of papers per simulator displayed by Scopus database between 2020 and 2023, under our constraints. Software with the same number of publications are grouped together.

scientific literature (37%, 13% and 10%, respectively). The ML initial search displayed 115 hits. Once a refined search was undertaken by adding the word “modelling”, the number was reduced to 41. Note that these numbers are current to 2024 and the authors anticipate these numbers to increase rapidly in the coming years.

The second step included using the three filters discussed in the previous section. The number of software-related and machine learning publications was hence reduced to 94 and 23, respectively. It is worth noting that, with regards to geothermal reservoir modelling, the earliest ML paper that fits our search dates from 2017. The number of papers in this field has increased significantly since 2021 (Figure 1a). A null result in the years 2018 and 2019 is consistent with the review by Pugliese *et al.* (2021) and Okoroafor *et al.* (2022) as shown in Figures 1b and 1c, respectively. From three databases: PubMed, Web of Science, and ScienceDirect, Pugliese *et al.* (2021) selected all published documents (i.e., journal papers, reviews, conference papers, preprints, code repositories and more). The following keywords were used in their Boolean search: "machine learning" OR "machine learning-based approach" OR "machine learning algorithms". Okoroafor *et al.* (2022) provided insights into ML subsurface applications in geothermal by searching both conference and journal papers in the IGA’s database and Google Scholar. AI-related keywords in the publications’ titles were used in the search by Okoroafor *et al.* (2022). These keywords were: "artificial intelligence", "machine learning", "deep learning", "statistical learning", "supervised learning", "unsupervised learning", and "neural network".

Compared to the two aforementioned works, the present study focuses on a shorter time range. Additionally, by using AND as a Boolean and “machine learning” as the sole keyword, fewer papers are considered. This is consistent with the purpose of the study: to identify how geothermal reservoir modelling can contribute to meet the COP28 commitment of tripling its output by 2030. The third step of the software-related search involved grouping the papers into one list per simulator for a total of 20 lists (See Figure 2) where 92 papers were identified. Given the clear dominance of COMSOL and TOUGH2 in the results, 53 papers associated with these simulators were chosen as eligible for the review. The number of COMSOL and TOUGH2 related papers is rather constant through the 4 years analysed here (15

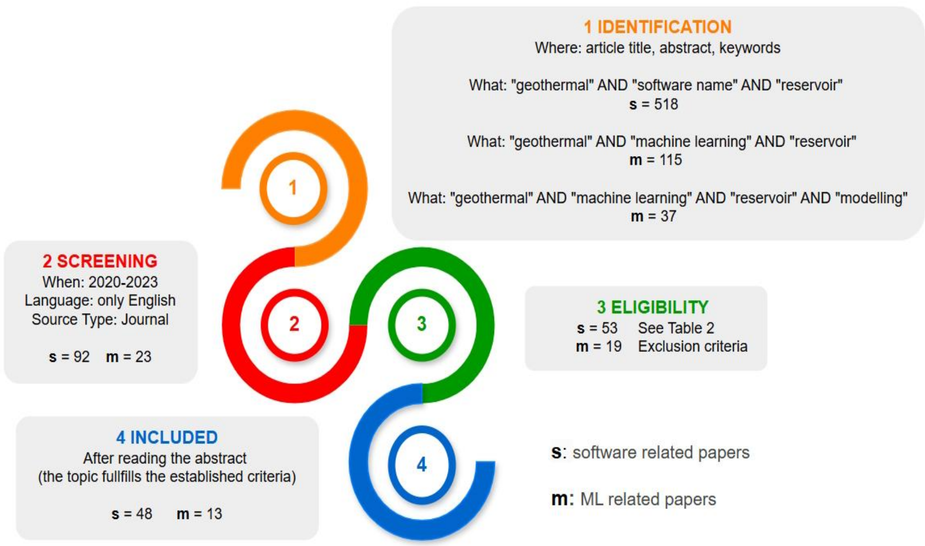

Fig. 3. Flow diagram of search strategy for literature review. Number of papers for: software (s) and machine learning (m).

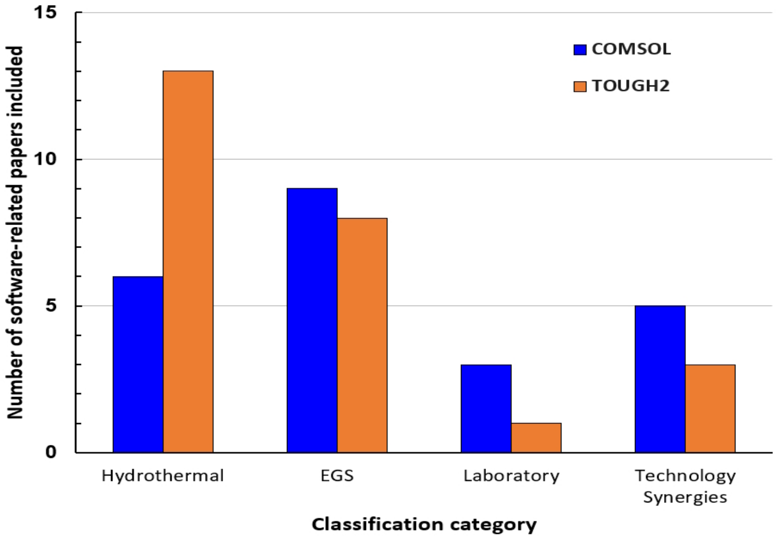

Fig. 4. Classification categories for software-related papers included

in 2020, 16 in 2021, 13 in 2023), with a small decrease in 2022, when only 9 papers have been published in journals indexed in Scopus. 21 ML papers were identified after discarding two manuscripts not related to geothermal.

The exclusion criterion applied in the last step required papers to address geothermal subsurface reservoir modelling. This resulted in several citations being excluded on screening the titles, keywords and abstracts. Subsequently, 48 software (23 COMSOL and 25 TOUGH2) and 13 ML papers were included in this review and the findings discussed in Section 3. The 4-step search strategy applied to decide on the articles to undertake the scoping review as described above is summarised in Figure 3.

2.4. *Analysing and charting the data*

The analysis of findings was conducted under a combination of both application-driven and theory-driven approaches. Laboratory experiments allow measuring parameters that cannot be made in the field. The field experiments complement the laboratory data by allowing mapping and testing at larger scales. However, both approaches have their limitations and as a consequence the laboratory and field results provide a motivation for numerical and theoretical models to explore the fundamental physics of processes. For this stage the categorization of manuscripts follows the global geothermal market and technology assessment by IRENA and IGA (2023).

The most widely developed geothermal energy resources are found in hydrothermal reservoirs, which consist of hot fluids circulating through deep permeable rocks. Nevertheless, EGS applications were identified as a recurrent theme that emerged from the papers, so its category has been included. Geothermal is synergistically expanding into cross-industry projects such as: oil and gas, mineral recovery, harnessing geothermal potential of abandoned mines, and Carbon Capture and Storage (CCS). Other examples of collaborative applications include Advanced Geothermal System (AGS), which involves closed loop heat exchangers and electricity generation, and Thermal Energy Storage (TES), which combines climatization technology with underground heating or cooling resources. Therefore, in defining geothermal applications, the work discussed in the software-related articles was classified into: hydrothermal, EGS, laboratory, and technology synergies (Figure 4). As ML is not a software, the analysis of the findings was completed separately.

3. Findings

3.1. *Published works after COP25*

The search was conducted for each software listed in Table 1. As shown in Figure 2, a total of 92 software-related papers satisfied the three filters discussed in Section 2.2. These data show that between 2020 and 2023, under the constraints of this work, 56% of the published modelling work cited TOUGH2 and COMSOL. In particular, the number of papers using these two simulators is at least 20 higher than any of the other softwares

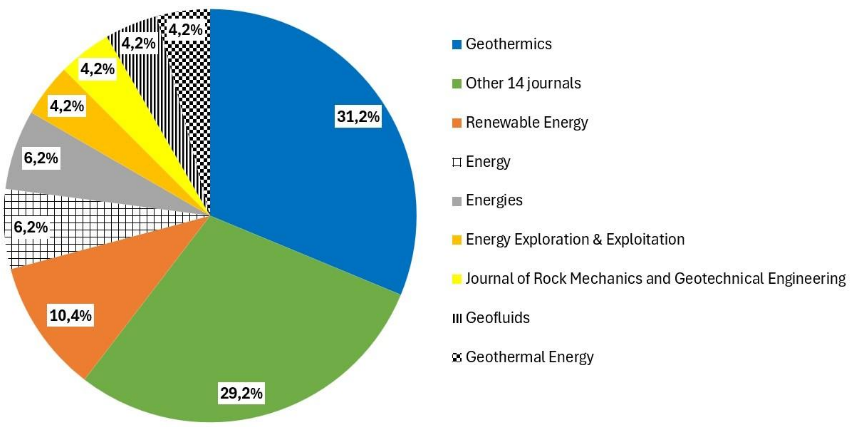

Fig. 5. Combined pie chart analysis of journals by numbers of published COMSOL and TOUGH2 papers included in this review.

Table 2
Journals with one paper published.

Journal	Software
Processes	TOUGH2
Applied Energy	
Water Resources Research	
Natural Resources Research	
Geoenergy Science and Engineering	
Journal of African and Earth Sciences	
Journal of Groundwater Science and Engineering	
International Journal of Rock Mechanics and Sciences	
International Journal of Rock Mechanics and Mining Sciences	
	COMSOL
Sustainability	
Energy Reports	
Rock Mechanics Bulletin	
International Journal of Mining Science and Technology	
Energy Sources Part A Recovery Utilization and Environmental Effects	

(Figure 2). The usage is suggesting that TOUGH2 and COMSOL can address the current demand and specific problems of trending interest. TOUGH2 is well-known as a popular simulator in the geothermal industry (Burnell 2012; Nugraha *et al.*, 2022). The finding about a recent preference for COMSOL for geothermal purposes is an outcome of this search. The remaining 44% of the manuscripts describe modelling studies conducted with the other 20 software packages. This is not to say that they do not have the appropriate modelling capabilities, but under the constraints of this work are not considered.

After applying the exclusion criterion, the 48 software-related papers included in this review were published in 22 different journals (Figure 5). Geothermics led with 31.2% of manuscripts followed by Renewable Energy with 10.4%. The segments with solid colour correspond to journals publishing both COMSOL and TOUGH2 papers, as also shown later in Figure 6. In contrast, the segments with patterned filling indicate those journals where only COMSOL papers were published. The 14 journals (29.2%) mentioned in Figure 5, where one paper per journal was published, are shown in Table 2 along with the related simulator.

Figure 6 shows that should this analysis be done separately for COMSOL papers, Geothermics and Renewable Energy share the second place with 17.4% each. In contrast, Geothermics

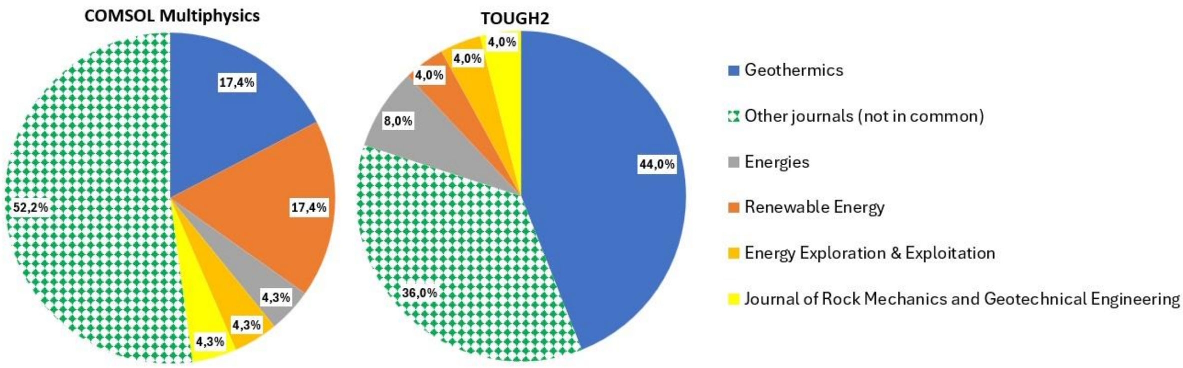

Fig. 6. Pie charts analysis for journals where COMSOL and TOUGH2 papers included in this review were published.

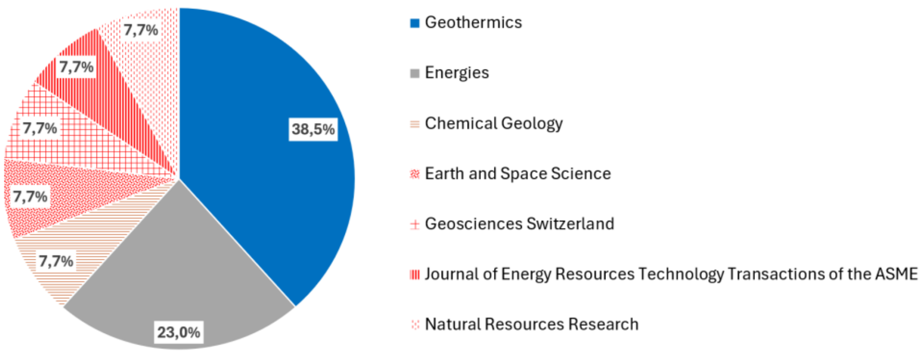

Fig. 7. Chart analysis for journals where ML-related papers included in this review were published.

remains the preferred option when reporting on TOUGH2 works with 44% while 4% appeared in Renewable Energy. With regards to the journals where ML papers were published among seven journals, as seen in Figure 7, Geothermics remains the preferred choice (38.5%), followed by Energies (23%).

3.2. Top 2 most frequently reported simulators under the constraints of this search

3.2.1. TOUGH2

Thermo-Hydro-Mechanical (THM) modelling of EGS processes was a common topic of interest (Zareidarmiyan *et al.*, (2020), Zhu *et al.*, (2023), Yu *et al.*, (2023), Liu *et al.*, (2023)). EGS long-term fluid injection is usually linked to induced seismicity. However, TOUGH2 simulations with Equation of State for pure water (EOS1) by Schiavone *et al.* (2020) showed withdrawal-reinjection is considerably less critical than simple injection. Zareidarmiyan *et al.* (2020) also investigated effects of water injection into naturally fractured rocks using CODE_BRIGHT and TOUGH-UDEC. The dissimilar results highlighted the challenge of accurately modelling the highly nonlinear nature of fractured rocks. Wang *et al.* (2020) introduced an Embedded Discrete Fracture Method (EDFM) that can be implemented in TOUGH2-EGS. EDFM allows incorporation of arbitrary discontinuities. The accuracy of this approach for heat transfer simulation seems more challenging than fluid flow in the porous medium. This is due to the thermal diffusivity being typically two or three orders of magnitude smaller than the fluid diffusivity. On the other hand, Yu *et al.* (2023) used TOUGH2-EGS and focused on hybrid fracture patterns which were treated as one continuum of Multiple INteracting Continua (MINC). A combined Extended Finite Element Method (XFEM) and EDFM-MINC Model handled arbitrary fracture shapes. Fracture aperture was opened by the cold fluid injection and reservoir performance was dominated by the thermal stress/strain. Liu *et al.* (2023), coupled an analytical/laboratory study to investigate THM processes. A multi fractured model validated through compression tests on Beishan granite was used to model the Rittershoffen EGS project (France). Their analysis accounted for the impacts of microcracks and fracture variations in the macroscopic deformation, permeability and thermal conductivity of saturated fractured rocks under coupled loading. In terms of EGS economic feasibility, Zhu *et al.* (2023) considered that a complete study must include both the connectivity of the artificial fracture network and the most efficient energy production mode. Their random fractured TOUGH2-BIOT model showed the Chinese Matouying reservoir's fracture network forms in three stages: conducting discontinuities' hydraulic aperture reaches a maximum; conductivity is achieved by fractures overcoming in situ stress; rock undergoes shear failure: the fracture expands and connects. Double vertical wells showed the highest outlet temperature while horizontal wells had the highest heat power output and heat extraction rate. Similarly, Ma *et al.* (2022) used 3DEC code and TOUGH2-EOS1 estimated permeability values, to analyse the heat production performance of the Zhacang project in the Guide Basin (China). This field was also modelled by Liu *et al.* (2020a). However, there was not enough field data to calibrate the Discrete Fracture Network (DFN) model. The results were compared to equivalent heat from coal. TOUGH2-EOS1 was also used by Zeng *et al.* (2021) to study the factors affecting the production performance of the Gonghe Basin (China). The results showed that decreasing well spacing and increasing fracture spacing reduces the electric power and energy efficiency with minimum impact on reservoir impedance. Increasing fracture permeability, however, improves the energy efficiency, reduces reservoir impedance resulting in more stable electric power production over time.

The Iceland Deep Drilling Project (IDDP) aims to produce supercritical (Sc) hydrothermal fluids as an economic geothermal energy source. Battistelli *et al.* (2020) used wellbore and reservoir characteristics of the IDDP-1 well in the Krafla field, to improve the EOS2 module for simulating H_2O-CO_2 mixtures. This was possible by including the capability to model thermodynamic conditions of Sc-steam-like reservoirs. The improved module coupled with the wellbore-reservoir simulator (T2Well-EOS2H) was successfully verified against results from iTOUGH2-EOS1Sc, STAR-HOTH2O, AUTOUGH, T2Well-EWASG and PROFILI. Comparatively, Feng *et al.* (2021) developed an EOS module for simulating Sc-reservoirs. Multiphase flow and behaviour between sub- and Sc-geothermal conditions were considered. A 1-D vertical column model was used, and findings were applied to the IDDP-2 well conditions to assess its production. Excessive reservoir temperature was deemed to lower the mobility of Sc-water resulting in an early thermal breakthrough. An updated Krafla field model was presented by Scott *et al.* (2022). The natural state temperatures from 40 wells, including IDDP-1, were used. ML techniques were applied for calibration and the results suggest the existence of an undeveloped resource. A model by Aydin and Akin (2021) used data from more than 100 wells of the Alaşehir field (Turkey), developed by seven operators. The model was used to identify potential problems for harnessing the resource. The results agreed with a Monte Carlo simulation and suggested unitized reservoir management as the best option to maximise production. Also in Turkey, a preliminary study for the Yerköy hydrothermal reservoir was undertaken by Yilmaz Turali and Simsek (2023). Monte Carlo simulations results by Lesmana *et al.* (2021) were compared with TOUGH2 runs for the Field Development Plan (FDP) of the Tompaso field (Indonesia). The proven reserve was calculated using the Box-Behnken experimental design and dynamic deliverability method. Forecasting suggested that using a stepwise development strategy can reduce the required amount of reinjection and make-up wells. An FDP for the Indonesian Patuha project was presented by Pratama *et al.* (2021). The Patuha reservoir's top part is steam dominated, while hot liquid water occupies the bottom. TOUGH2 was used to simulate the effects of the Dry-Steam Cycle Unit (DSCU) and the Integrated Geothermal Combined-Cycle Unit (IGCCU) on reservoir production sustainability. The higher injection rates into the brine zone from IGCCU yielded higher electrical power generation than DSCU. Continuing with the volcanic reservoirs, Seyedrahimi-Niaraq *et al.* (2021a) used EOS3 to model the Sabalan field (Iran), which was classified as medium-enthalpy liquid-dominated. This project's power production capacity was estimated by Seyedrahimi-Niaraq *et al.* (2021b) through an improved EOS1 module validated with data from 10 exploration wells. The forecast showed production capacity was controlled by drops in pressure and production fluid enthalpy. In Russia, near the Koryaksky volcano, a model of the thermal and water recharge of the Ketkinsky field was proposed by Kiryukhin *et al.* (2022). iTOUGH2-EWASG simulations of the natural state and modelling of the hydrodynamic production history was used to estimate the thermal fluid upflow, permeability and compressibility. Forecast scenarios confirmed the possibility of the field's sustainable operation. Tescione *et al.* (2021) built simulations contrasting previous conceptual models of the Torre Alfina medium enthalpy field, near the Bolsena Caldera (Italy). The reservoir was interpreted as being mostly recharged by lateral advection of heat and fluids from the caldera deep high-enthalpy resources, through permeable faults. Guerrero *et al.* (2023) updated the conceptual model of the Las Tres

Vírgenes hydrothermal field (Mexico) and ran EOS3 simulations. A rough temperature match was obtained and well test and early production data were recommended for model calibration. Faraz *et al.* (2021) proposed a Local Thermal Non-Equilibrium (LTNE)-based formulation and results compared to AD-GPRS and TOUGH2. The LTNE model made the simulation more accurate. If a boiling regime is expected to develop, it may be useful considering boiling heat transfer.

Three papers addressed cross-industry applications. Xu *et al.* (2020) used T2Well to investigate the heat extraction performance of co-axial geothermal closed-loop processes. The findings discuss the benefits of intermittent production cycles for heat extraction and maintenance. Additionally, Xu *et al.* (2020) found higher production temperatures and lower heat extraction rates were directly proportional to increments in the injection temperature. While permeability and porosity had little effect on productivity, higher heat conductivity and geothermal gradients led to higher output temperature and overall influence on the closed-loop performance. Ezekiel *et al.* (2020) proposed $ScCO_2$ as a working fluid for Enhanced Gas Recovery (CO_2-EGR) and extracting geothermal energy (CO_2-Plume Geothermal – CPG) from natural gas reservoirs, while ultimately storing the injected CO_2. Simulations with EOS7C coupled to a wellbore heat-transfer model confirmed its technical feasibility. Modelling of this combined technology by Ezekiel *et al.* (2021) showed the natural gas recovery performance was most sensitive to permeability anisotropy and reservoir temperature. The geothermal power generation performance, on the other hand, was deemed most susceptible to reservoir temperature and production wellbore diameter. Of these two, reservoir temperature has between five and ten times greater beneficial effect on the power output than any other parameter evaluated.

3.2.2. COMSOL

This review shows that COMSOL is widely used to provide a better understanding of EGS behaviour, through the simulation of coupled THM processes. In particular, simulations focused on 1) validation of numerical models with field data from the Fenton Hill HDR test site in New Mexico (Aliyu and Archer, 2021a); 2) analysis of the impact of wellbore alignment and placement, with single and multiple planar fractures. This includes the effects of fracture spacing and number on: production temperature, recovery, and thermal extraction rates (Aliyu and Archer, 2021b); 3) study of the effect of cold fluid circulation and the consequent rock contraction, causing the thermoelastic effect on fractures (Aliyu *et al.*, 2023); and 4) investigation of the impact of heat recovery capability of: injection water temperatures and rates; injection-production pressure differentials; and reservoir's initial temperature (Wang *et al.*, 2023). Simulations were also applied at the wellbore scale to predict temperature and heat loss within the GPK-2 production well of the operating EGS at Soultz-sous-Forêts in Alsace (France) (Akhmetova *et al.*, 2023). The papers included in the EGS category also provided an overview of alternative approaches to represent fractured reservoirs. Liu *et al.* (2020b) for instance, combined thousands of small fractures, randomly generated with the natural discontinuities identified through field investigations. From this, a 2D geological model of the fracture network was built for the granite of Sanguliu area located in the Liaodong Peninsula, Eastern China. McLean and Espinoza (2023) pursued a more complex model for an EGS project. They used 2D fractures embedded in a 3D porous rock intersecting production and injection wells to study the influence of thermo-poroelastic interaction on decreasing the system's performance. They compared two scenarios with 2 and 5 fractures and demonstrated that thermal short-circuiting occurs earlier when more fractures are considered. This is due to the thermal and mechanical interaction of the fractures. Hu *et al.* (2022) worked with between 5 and 15 discrete horizontal fractures for the production of heat required for oil sands separation in Alberta, Canada. Specifically, they compared the performance of doublet and triplet EGS configurations. Aliyu and Archer (2021a; 2021b) built a 3D reservoir model with few vertical fractures (< 10). This was based on data from the Fenton Hill HDR site. Wang *et al.* (2022) built a model with a single horizontal fracture, intersected by production and injection wells, while Wang *et al.* (2023) considered 2 discrete fractures (vertical and horizontal) as the main pathways for heat transfer.

The use of COMSOL for the modelling of hydrothermal reservoirs is not as common as it is for EGS (Qarinur *et al.*, 2020). However, the simulation of the reservoir's natural state, before production, is required to quantify the impact of fluid extraction and ensure sustainability in hydrothermal fields. One such field is the Lahendong geothermal field, in North Sulawesi (Indonesia) investigated by Qarinur *et al.* (2020). A different type of hydrothermal resource was modelled by Aguilar-Ojeda *et al.* (2021a), to improve the understanding of the submarine hydrothermal vent in the Maneadero geothermal field (Mexico). Wang *et al.* (2021) studied the injection of low-temperature tail water into a carbonate reservoir in the geothermal field of Xian County (China), highlighting that reinjection pressure, temperature and well spacing are the main factors for the control of geothermal production and reinjection. Another key factor for optimal reservoir management is the change in porosity. For example, Thermo-Hydro-Chemical (THC) coupling was applied to model the combined effects of porosity reduction and generation of enthalpy caused by silica precipitation (Gisler and Miller, 2021). Liu *et al.* (2022) also used THC simulations, but focused their study on the prediction of the thermal breakthrough of production wells in the Xianxian geothermal field (China). Numerical simulations can also be used to assess the economic output of geothermal production, as done by Daniilidis *et al.* (2020). They analysed the lifetime, generated Net Present Value, and produced energy of single doublet within a faulted block, in a conduction dominated sedimentary geothermal reservoir. The effects of varying the well spacing and placement, reservoir layers, fault properties, injection and production flow rates were studied.

COMSOL was also used to model laboratory-scale experiments. Kumari and Ranjith (2022) investigated the impacts of water viscosity and density reduction on Australian Strathbogie granite cylindrical specimens under high-temperature and pressure triaxial conditions. They predicted permeability, pressure and strain under extreme conditions. Additionally, thermal shock and fatigue on the rock mass on granite cuboid samples collected at outcrops at Xinjiang (China) were studied by Hu *et al.* (2021). They provided a better understanding of the variation of rock properties and heat transfer performance after thermal damage. Finally, a large sandbox experiment was conducted by Li *et al.* (2023) to investigate the internal temperature evolution in a sandstone aquifer under different reinjection scenarios, considering THC coupling. Quantifications of the impact of the reinjection temperature, rate, and well spacing on the thermal breakthrough time of the production well were offered.

Insights into geothermal reservoir simulation trends include the growing interest in recent technologies. Among AGS, coaxial borehole heat exchangers are seen as an option to reuse depleted petroleum wells in Alberta (Canada) (Hu *et al.*, 2020), and also to unlock the EGS resources in the Matouying uplift in Northern China (Niu *et al.*, 2023). With this technology, several parameters show an impact on the heat extraction performance. These include inlet temperature and flow rate, the thermal conductivities of the cement, the inner tube and the reservoir borehole diameter, fluid de-circulation mode, and geothermal gradient (Niu *et al.*, 2023). However, significant debate still remains as to the feasibility, performance, and cost competitiveness of AGS, for either co-axial or U-loop systems, analysed with the GEOPHIRES v2.0 techno-economic assessment tool (Beckers *et al.*, 2022).

Underground water storage and heat production from abandoned mines is increasingly being considered for energy savings and emissions reduction. One such example is the Jiahe abandoned coal mine modelled by Guo *et al.* (2023). Another is Thermal Energy Storage (TES). Among all the available TES options, the use of Aquifers (ATES) is widely used in some places, such as The Netherlands, China, and North America, as mentioned by Stober *et al.* (2023). These authors also presented a case study in the Buntsandstein aquifer, in the Upper Rhine Graben (Germany).

3.3. The role of Machine Learning (ML)

ML is a subcategory of artificial intelligence that allows computers to train from data, without requiring specific-purpose programming. A subset of ML is Deep Learning, which is based on neuronal networks. For the sake of clarity, hereafter both Deep Learning and ML will be referred to as ML algorithms. These are usually applied to subsurface reservoir modelling given their great potential for emulating computationally intensive components of numerical simulations using surrogate models (Rajabi and Chen 2022; Collard *et al.*, 2023). Jiang *et al.* (2022) stated that data-driven models have less complexity than the traditional numerical models, although the latter offer the most comprehensive dynamic approaches. In fact, ML methods allow for a quick estimation of reservoir variables.

Duplyakin *et al.* (2022) showed that while a typical reservoir simulation run takes approximately 4 hours to complete; the corresponding ML model yields accurate 20-year predictions for temperatures, pressures, and produced geothermal energy in 0.9 seconds. Since available geothermal field data are usually not enough to provide a training set for ML, the numerical physics-based reservoir simulations can be used to generate those data sets (Rajabi and Chen 2022; Duplyakin *et al.*, 2022). Abrasaldo *et al.* (2023), for example, developed a workflow combining data analytics and numerical reservoir models with TOUGH2 to analyse the behaviour of weak production wells. Suzuki *et al.* (2022) explored the use of ML methods for inverse analysis in reservoir modelling, a task that is usually computationally expensive when using traditional tools such as iTOUGH2, UCODE and PEST. Duplyakin *et al.* (2022) used TETRAD and STARS to generate a training data set for ML algorithms, using a synthetic, yet realistically data-populated, reservoir. This was specifically built to feature the Brady Hot Springs in Nevada (USA), where there is an operating geothermal power plant. TETRAD was also used by Jiang *et al.* (2022) for short and long-term prediction of energy production from a synthetic geothermal field. Gudala and Govindarajan (2021) built a THM model with COMSOL and trained and validated 6 ML algorithms to predict production temperature considering changes in reservoir´s pressure, temperature and geomechanics as well as the rock´s physical, mechanical and thermal properties. In summary, these studies demonstrated the utility of ML algorithms for predicting reservoir performance without the need for intensive computational effort, through their combination with traditional numerical modelling software.

The implementation of ML tools helps reservoir exploration, characterization, and management: from the estimation of properties distribution at reservoir scale, such as permeability (Suzuki *et al.*, 2022; Zhang and Wu 2023) and mineralogical composition (Hu *et al.*, 2023) to the optimisation of the management of geothermal reservoirs (Abrasaldo *et al.*, 2023; Duplyakin *et al.*, 2022; Jiang *et al.*, 2022; Rajabi and Chen 2022; Gudala and Govindarajan 2021). Zhang and Wu (2023) applied an optimised version of the deep belief network (DBN) model to predict the permeability of the sandstone reservoir of the Baiyanghe Formation in the geothermal field of Zhangye Basin (China). Hu *et al.* (2023) used a hybrid ML architecture to describe the mineralogical compositions from well logs from the Horn River Basin, northeast British Columbia (Canada). Another relevant example is the application of ML to maximise the Rate of Penetration (ROP) and hence reduce geothermal drilling costs: Ben Aoun *et al.* (2022) used data from the FORGE field laboratory in Utah (USA) to collect drilling data such as the ROP,

Table 3
ML algorithms used in the papers included in this review.

Research Area Topic	**ML Algorithm (Reference)**
Exploration	
Play Fairway Analysis	BNN, PCAk (Smith *et al.*, 2023)
Depleted oil and gas reservoirs	GFCM (Topor *et al.*, 2023)
Drilling	
Maximisation of the ROP	RF, ANN (Ben Aoun *et al.*, 2022)
Reservoir Characterization	
Geochemical databases	DT, SVM, RF (Santamaría-Bonfil *et al.*, 2022)
Reservoir permeability distribution	LR, SVR, MLP, RF, gBoost, KNN (Suzuki *et al.*, 2022)
Reservoir permeability distribution	DBN (Zhang and Wu, 2022)
Hydrothermal dolomitization	RF, GBoost, AdaBoost, SVM, MLP (Collard *et al.*, 2023)
Mineral composition	CNN, XGBoost (Hu *et al.*, 2023)
Production and Injection Well Engineering	
Low permeability wells	RF, gBoost (Abrasaldo *et al.*, 2023)
Energy production	RNN, FCNN, LSTM (Jiang *et al.*, 2023)
Optimization of energy production	NN (Duplyakin *et al.*, 2022)
Simulation-optimization	NN, CNN, RNN, RF (Rajabi and Chen, 2022)
Reservoir Engineering	
THM modelling	LR, SGD, DT, RF, SVM, DNN (Gudala and Govindarajan, 2021)

weight on bit, temperature, and pump pressure. The ML tool created from these data enabled better selection of drilling parameters for the FORGE site. This validates the usefulness of ML algorithms in reducing the risks associated with drilling, one of the main barriers to geothermal field development.

Considering geochemistry, ML algorithms were employed to fill the gaps in a geochemical database of geothermal fluids based on literature available data from 140 geothermal sites located in twenty-five countries (Santamaría-Bonfil *et al.*, 2022). The outputs from this exercise were used to predict dissolution and precipitation of calcite and dolomite, which can enhance or reduce reservoir porosity (Collard *et al.*, 2023). Distinct applications of ML were the improvement of Play Fairway Analysis for geothermal potential maps in the Great Basin region of Nevada (Smith *et al.*, 2023) and the identification of high potential in two depleted oil and gas reservoirs in Poland (Topor *et al.*, 2023).

Based on the classification suggested by Okoroafor *et al.* (2022), Table 3 shows most of the reviewed ML studies addressed the topics of reservoir characterization and production/injection well engineering. Considering that drilling is the most crucial phase in the development of a geothermal power project, and only one study (Ben Aoun *et al.*, 2022) was identified under the constraint of this search, this is a possible field for further research.

Also shown in Table 3, mainly Neural Networks (NN) and Random Forest (RF) were applied in the reviewed studies. Among NN, several variants were mentioned: Artificial (ANN); Recurrent (RNN); Fully Connected (FCNN); Bayesian probabilistic (BNN); Inversion (INN); Convolutional (CNN); Physics-Informed (PINN); Long Short-Term Memory (LSTM), and Deep Belief Network (DBN). LSTM is a particular type of RNN, which is designed to learn long-term dependencies. Other tools were the Linear Regression (LR) and its variants for model regularisation (ridge and Lasso), Support Vector Regression (SVR), Multi Layer Perceptron (MLP), Stochastic Gradient Descent (SGD), Decision Tree (DT), Gradient Boosting (gBoost), eXtreme Gradient Boosting (XGBoost), Adaptive Boosting (AdaBoost), K-Nearest Neighbors (KNN), Support Vector Machines (SVM), Generalised c-Means (GFCM), and Principal Component Analysis paired with k-means clustering (PCAk).

4. Discussion

4.1. Bibliometric trends as pointers to future directions

Biblioshiny is a web-based interface for the open-source R package *bibliometrix* (Aria and Cuccurullo, 2017). *KeyWords Plus* are words or phrases that appear in the titles of a manuscript's references, but not in the title of the document itself. Figures 8-

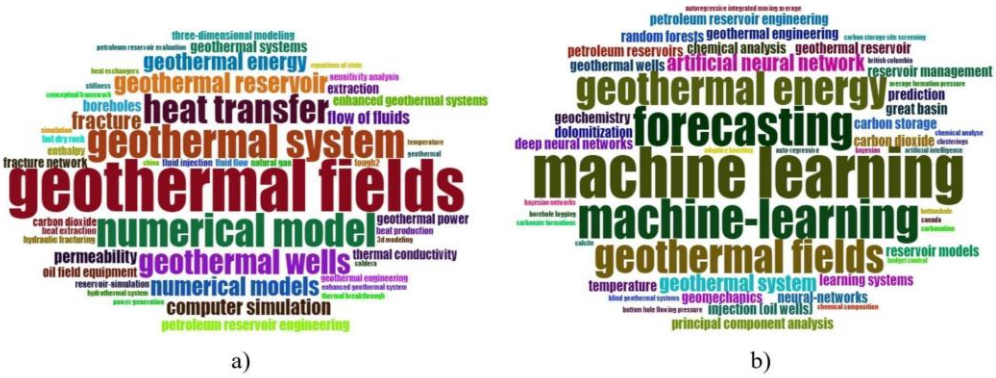

Fig. 8. Word cloud comparison using KeyWords Plus for papers on: a) TOUGH2+COMSOL and b) ML

Fig. 9. Co-occurrence density plot for KeyWords Plus for (a) TOUGH2+COMSOL and (b) ML+software-related papers included in this review.

10 allow analysing these text data within the context of scientific published trends. Figure 8 displays the most frequently used terminology by font size in word clouds. Figure 9 depicts *KeyWords Plus* co-occurrence in the same paper in the form of density plots. Figure 10 shows the interrelationship between authors' research topic, country, and affiliation. In three-field diagrams, the size of the rectangle in each list indicates the number of manuscripts associated with an element.

Figure 8 depicts a word cloud comparison of the 48 publications on TOUGH2/COMSOL (Figure 8a) versus 13 papers on ML (Figure 8b). The visualisation illustrates a prominent focus on "heat transfer" and "forecasting" when using software or ML, respectively. The modelling of fractured media with simulators seems to be an actively studied topic as highlighted by "fracture", "EGS", "fracture network", "permeability" and "hydraulic fracturing". Key ML themes encompass "geochemistry," "dolomitization" and "chemical analysis." These align with major research findings, accentuating the challenge of fully coupled THMC simulations in geothermal reservoirs. Among ML algorithms, neural networks are the most cited. Oil and gas is a common topic, and demonstrates the skills transferability and adaptability to geothermal resources. Finally, carbon dioxide appears in both clouds showing industry synergy with geothermal.

To highlight the impact of ML compared to traditional numerical models, Figures 9 and 10 also include a combined representation, i.e. software + ML-related papers. The relevance of "numerical model" (underlined in cyan in Figure 9a) seems more impactful than when the ML papers are included in the visualisation (Figure 9b). Instead, the word 'forecasting' rises within a new cluster (inside the green ellipse). This suggests that ML algorithms could be used to improve accuracy and by default reduce computational cost when combined with numerical models.

Figure 10a shows China is the leading country, with 7 institutes co-authoring COMSOL or TOUGH2 publications. This is followed by Mexico, Canada, Indonesia, USA, Iran, and Japan. Among the top 15 KeyWords Plus (Figure 10b), it is interesting to see that when the analysis includes the 13 ML papers, the keyword "petroleum reservoir engineering" rises in the list. This is most likely to do with the benefits of the findings of artificial intelligence inherited in geothermal from the oil and gas industry, as suggested by Okoraofor (2022).

Figure 11 shows that amongst the 61 manuscripts included for this review, the most cited paper was published by Hu et al (2020) titled "*Numerical modeling of a coaxial borehole heat exchanger to exploit geothermal energy from abandoned petroleum wells in Hinton, Alberta*". This was followed by the publication by Ezekiel *et al.*, (2020) titled "*Combining natural gas recovery and CO_2-based geothermal energy extraction for electric power generation*". The third most cited paper, "*Changes in the thermodynamic properties of alkaline granite after cyclic quenching following high temperature action*" was written by Hu *et al.*, (2021). Judging by these number of citations, two topics cover 70% of the top 10 most cited documents: EGS and the technology synergies. This observation indicates a trend in the modelling arena. The most referenced papers were published in Elsevier's *Renewable Energy*.

As its name indicates, open-source software are computer codes made available for use and/or modification by users. This allows public development and collaboration and could be a good alternative for spreading the benefits of modelling. From Table 1, eleven open-source software were identified: CFRAC, DARTS, Falcon, Geophires, Hydrotherm, OpenFoam, OpenGeoSys, PFlotran, Porepy, SUTRA and Waiwera. From this list, DARTS and Waiwera seemed to be the most used, with combined 26 modelling studies identified, representing 46%.

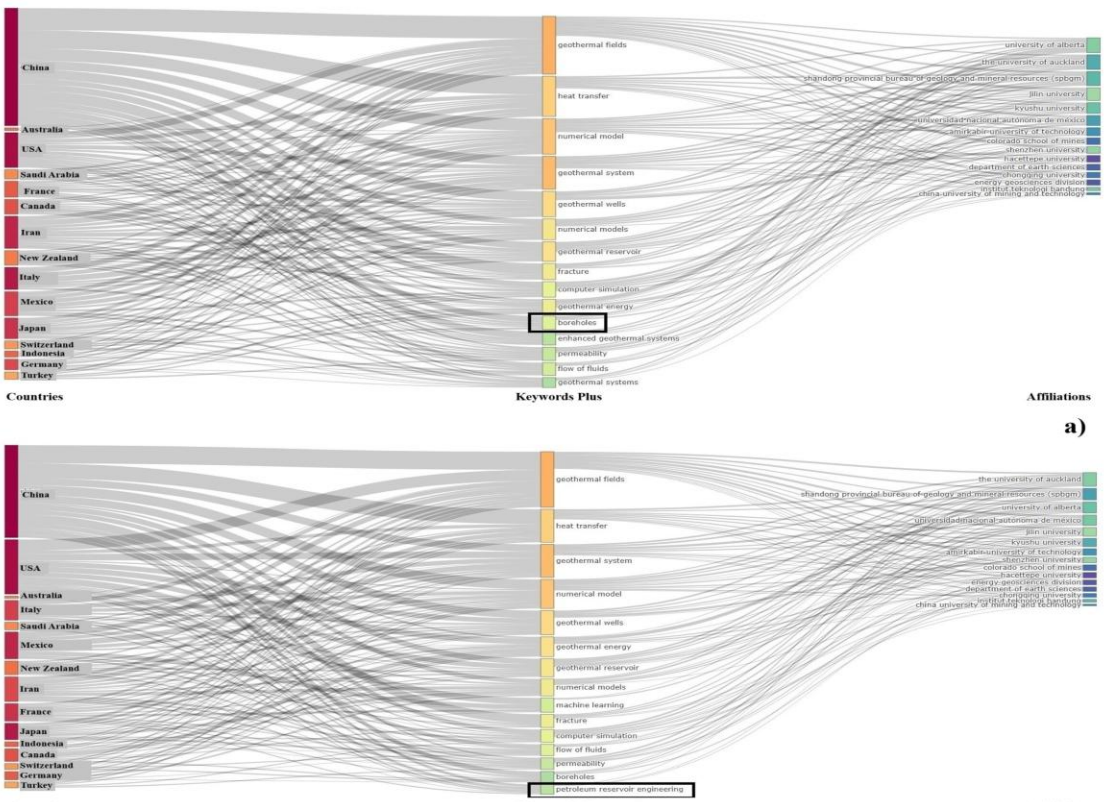

Fig. 10. Three-field plot showing per column the relation between Countries (left), KeyWord Plus (middle) and affiliations (right) for the a) COMSOL+TOUGH2 and b) ML+software-related papers included in this review.

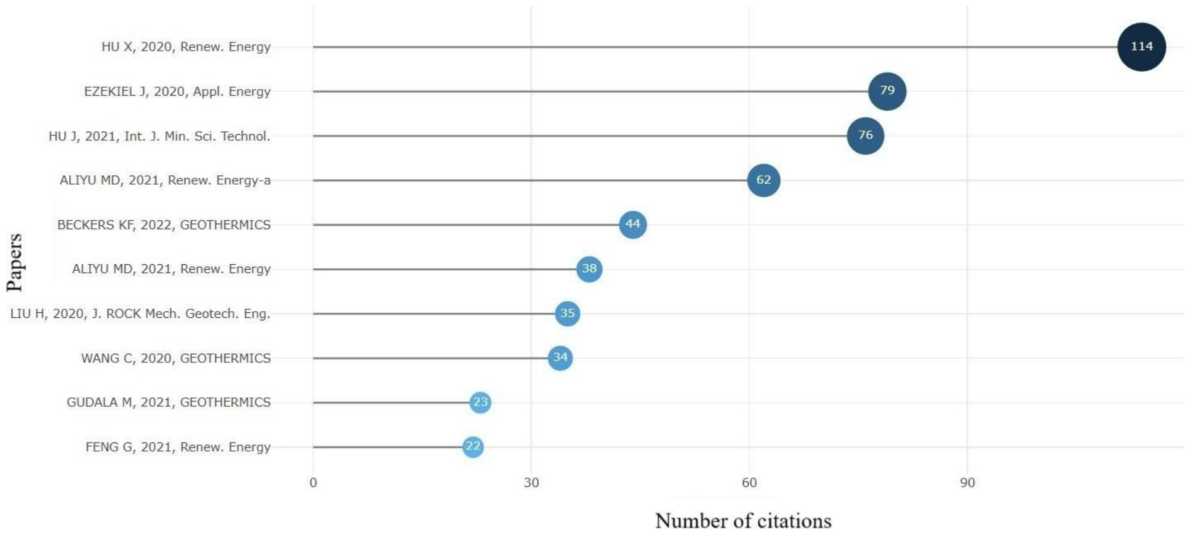

Fig. 11. Top 10 most global cited documents

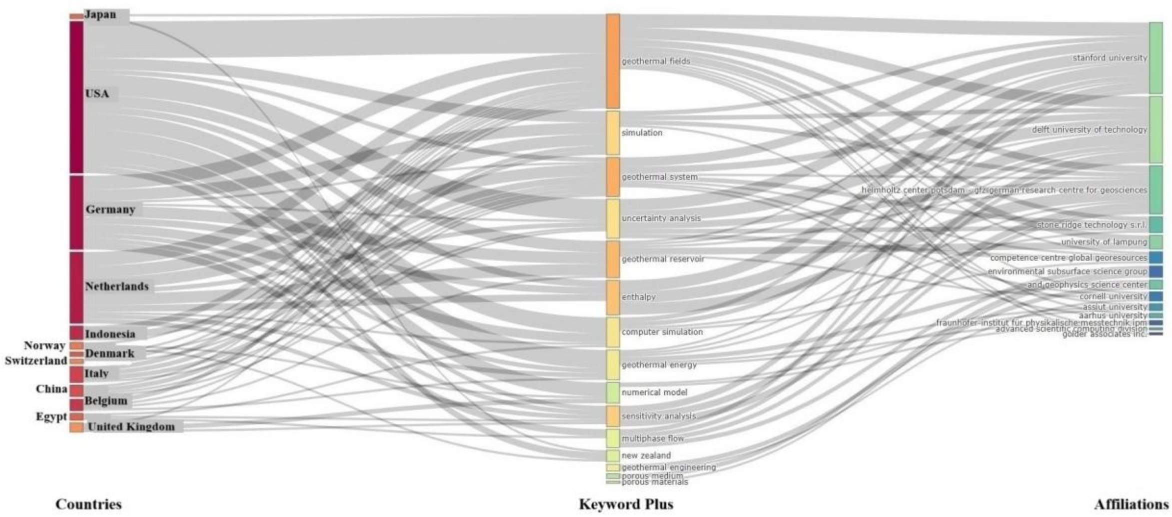

Fig. 12. Three-field plot showing per column the relation between Countries (left), KeyWord Plus (middle) and affiliations (right) for the Open-source simulators.

This number is comparable with the studies undertaken with TOUGH2 (25) and COMSOL (23).

Open-source applications are deemed more often employed in the United States and Europe (Figure 12), while TOUGH2 and COMSOL are mainly used in China (Figure 10). The three most cited documents from the open-source modelling studies (with 84, 70, and 46 citations respectively), are slightly less referenced than their equivalent to TOUGH2 or COMSOL (114, 79, and 76, Figure 11). However, the wide availability of open-source software offers a valid alternative to pursue research work especially in academia. Publications on models using open-source software are less cited than those undertaken with commercial software. However, given their low or null cost, they could be more affordable in countries with less economical resources.

4.2. TOUGH2 and COMSOL comparative analysis

Major advantages of COMSOL, over some software, include the capability to handle complicated geometrical structures, advanced and flexible mesh generation. In recent years, scripting has allowed easing of modelling automation, highly desirable for more complex simulations. The PyTOUGH library, for instance, enables users to potentially control simulation aspects from grid generation and model setup through execution, post-processing and analysis. A pythonic scripting interface is also available for COMSOL Multiphysics. The library is called MPh after the file extension of COMSOL models, which stands for multi-physics. MPh covers common scripting tasks, such as loading a model from a file, modifying parameters, importing data, to then run the simulation and results evaluation and exporting. Additionally, LiveLink™ enables integrating COMSOL with MATLAB to extend the users' modelling with programming in the MATLAB environment and use its toolboxes in preprocessing of data, model manipulation, and postprocessing. Likewise, iMatTOUGH supports the generation of inputs required for both TOUGH2 and iTOUGH2 and the output visualisation. A comparison of detailed capabilities of each simulator for the modelling of geothermal reservoirs is presented in Table 4.

Since 2020, developments for TOUGH2 include *toughio-dash*, a web application to simplify setting up TOUGH simulations. This provides a user-friendly graphical user interface and relies on the open-source Python library toughio

Table 4
Capability comparison between TOUGH2 and COMSOL for the modelling of geothermal reservoirs

Capability	TOUGH2	COMSOL
Fracture discretization	✓	✓
Normal stress- dependent fracture aperture	✓	✓
Shear-fracture aperture	✓	✓
Stress induced flow channelling	✓	✓
Porous flow in matrix	✓	✓
Thermo-elastic effects	✓	✓
Multiphase flow	✓	✓
3D	✓	✓
Flexible mesh generation		✓
Reactive transport modelling	✓	
Tracer transport	✓	
Phase displacement	✓	

and Plotly Dash. The EOS2H module has been developed to handle subcritical and steam-like supercritical H_2O-CO_2 mixtures. The newest version of COMSOL, Version 6.2, released in May 2024, increased the computational speed of their simulation apps using data-driven surrogate models.

Overall, COMSOL is considered a more user-friendly program, as highlighted in the recent work by Wang *et al.* (2023). Although the learning curve for TOUGH2 could be steeper, this suite of simulators has a larger applicability for large-scale complex fractured geothermal reservoirs. COMSOL can also be used to easily build models of geothermal well doublets and to introduce user-defined coupling equations. Fractured geological media can be more readily simulated with TOUGH2 than with COMSOL.

4.3. Insights from Machine Learning

According to Table 3, the 3 most used ML algorithms in the studies included in this review are NN, RF, and Boosting algorithms. Expert opinion, while not being unanimous, states that RF generally outperforms NN for small datasets (Qi 2012; Han *et al.*, 2021). However, different algorithms need to be assessed to select the best option for the specific problem analyzed (Ahmad *et al.*, 2017). The algorithm selection should be based on several criteria, such as its robustness, comprehensibility, and computational cost.

RF offers a balance between complexity and results. It uses multiple decision trees whose results are combined to obtain a single model, which is more robust compared to the results of each tree separately (Espinosa-Zúñiga, 2020). RF can handle missing data efficiently (Tang and Ishwaran 2017), but prediction can be slower than other algorithms. In contrast, Gradient Boosting algorithms focus on sequential correction of errors, since the learning algorithms are combined in series to achieve a strong learner ("boosting") from the individual decision trees connected sequentially (Di Salvo, 2022). Following this approach, XGBoost, for example, requires larger computational resources, but it has higher predictive accuracy than RF. Depending on the geothermal project stage (exploration, field development, and production), the quantity and quality of field data change. It is therefore recommended that ML algorithms are compared to identify the most appropriate, based on the available data and modelling purpose. Table 3 provides a useful guide for this selection.

Data scarcity, model validation, and computational constraints are key challenges for ML applications. Data scarcity can be a challenge when applying ML algorithms, since their predictions can be inaccurate, can fail in pattern recognition and can cause overfitting (Bobadilla, 2020). A detailed overview on strategies to tackle data scarcity in deep learning is offered by Alzubaidi *et al.* (2023). They highlighted that an initial large dataset improves the algorithm's ability to learn and identify patterns. They also mentioned a related challenge, which is data diversity. If the dataset included a variety of data types and sources, the algorithm can better generalize to new conditions and be reliable in real-world applications.

The validation methodology is based on the measurement of the model accuracy with a new dataset, to ensure the final product can handle new data (Bobadilla, 2020). The accuracy is the measure of correct predictions made by the model, after it has been trained. There is not a rule to establish the optimum ratio of training and validation data, but recent studies provide a guide (Di Salvo, 2022). This approach is similar to the validation of a numerical model, where field data different from those used for model calibration should be used for its validation.

The successful application of ML algorithms is based on the availability of a large amount of high-quality data. Therefore, data management and processing implies a high computational cost. This is demonstrated by the Department of Energy (DOE) of the United States that recently announced the colocation of data centers on its lands (DOE, 2025). The simplicity, fast run time, and acceptable accuracy of ML algorithms have made them popular. Recently, theory-guided machine learning, was applied to inverse modeling of groundwater dynamics (Adombi *et al.*, 2022). This new approach incorporates, during the training stage, certain constraints related to the governing equations describing a numerical model. By following this approach, ML algorithms do not deviate too far from the laws of physics. On the other hand, the link between ML algorithms and traditional numerical models is getting stronger with Reinforcement Learning (RL), an approach that introduces new mechanisms to cope with data scarcity (Duplyakin *et al.*, 2022). According to Di Salvo (2022), ML models do not offer a complete representation of the physical system and, thus, cannot be used to substitute traditional numerical models. Nonetheless, they can be used to improve predictions at specific locations, for better model calibration.

4.4. The role of numerical modelling

The last three subsections summarise the core concepts and findings covered in the literature included for this review. This decanting process involved understanding the paper's main arguments and the overall implications of the research. In order to distil this information into a concise form, a Venn diagram is used as a visual depiction (Figure 13). This graphic analysis maps three streams of work here compared, i.e. (i) geothermal numerical modelling, (ii) ML global trends and (iii) installed geothermal electricity capacity, in order to elucidate the needs

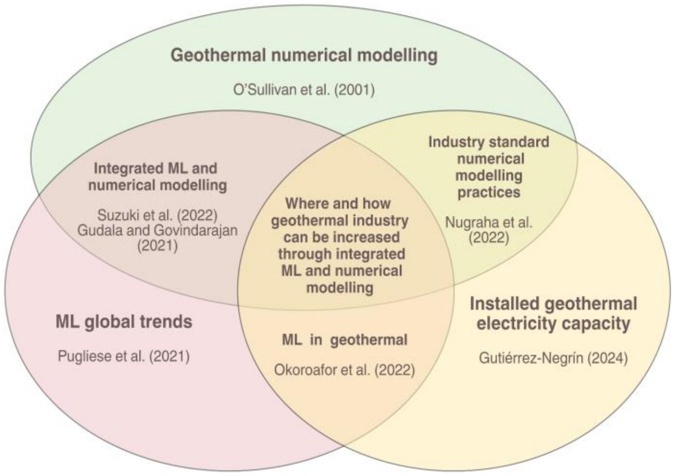

Fig. 13. Venn representation of the analysed contents, overlapping themes and identified needs.

to be addressed. The studies conducted by Suzuki *et al.* (2022) with TOUGH2, and by Gudala and Govindarajan (2021) with COMSOL were found to fit in the overlap between ML global trends and numerical modelling. The work of Nugraha *et al.* (2022) converges the topics of geothermal numerical modelling and power generation in operational geothermal fields. The third intersection is given by the review by Okoroafor *et al.* (2022), who identified a research area as production and injection, crucial to optimise the geothermal resource for power generation.

The significance of the overlapping of these streams is discussed in the following subsections taking into account geographical and policy insights. Suggestions for overcoming barriers for development are also proposed. Finally, a country case study is briefly presented, focusing on the economic, environmental and technical context to understand its unique challenges and opportunities for geothermal.

4.4.1. Geographical Insights

According to IRENA (2024a), in 2014 the world net generating capacity for geothermal energy was 11.25 GW. North America had the most with 3.38 GW, while Africa (0.373 GW) and South America (no installed capacity) were the two regions with the lowest geothermal development. Nine years later, the total world value rose to 14.85 GW, an increase of 32%. It is interesting to note that North America expanded its industry by 8.7%, while Kenya showed a growth of 166%, becoming a geothermal leader in Africa. As a matter of fact, as of December 2023, geothermal meets approximately 45% of Kenya´s total energy generation (EPRA, 2024). Gutiérrez-

Table 5
Most recent references about South American geothermal resources and data

Argentina
Geothermal Country Update of Argentina: 2015-2020 (Chiodi *et al.*, 2021)
Bolivia
Construction of Bolivia's first geothermal plant progressing (Cariaga, 2022)
Geothermal Development in Bolivia (Villarroel, 2014)
Brazil
Integrated assessment and prospectivity mapping of geothermal resources for EGS in Brazil (Lacasse *et al.*, 2022)
Present geothermal field of the Santos Basin, Brazil (Zuo *et al.*, 2023)
Chile
Heat in the news: Geothermal energy in Chilean newspaper coverage (Vargas Payera, 2024)
BrineMine-sustainable raw material and fresh water production from thermal fluids (Kählert, 2023)
Colombia
Approach to the geothermal potential of Colombia (Alfaro *et al.*, 2021)
Predicting the geothermal gradient in Colombia: A machine learning approach (Mejía-Fragoso *et al.*, 2024)
Ecuador
Geothermal resource exploration in South America using an innovative GIS-based approach: A case study in Ecuador (Jara-Alvear *et al.*, 2023)
Guyana
Guyana IRENA's energy profile (IRENA, 2024b)
Paraguay
Paraguay IRENA's energy profile (IRENA, 2024c)
Peru
Characterization of southern Peru hydrothermal systems: new perspectives for geothermal along the Andean forearc (Taillefer *et al.*, 2024)
Suriname
Suriname IRENA's energy profile (IRENA, 2024d)
Uruguay
Potential of geothermal energy in the onshore sedimentary basins of Uruguay (Morales *et al.*, 2021)
Venezuela
Approach to geothermal energy. A link additional for the Energy transition in Venezuela (Oquendo *et al.*, 2024)

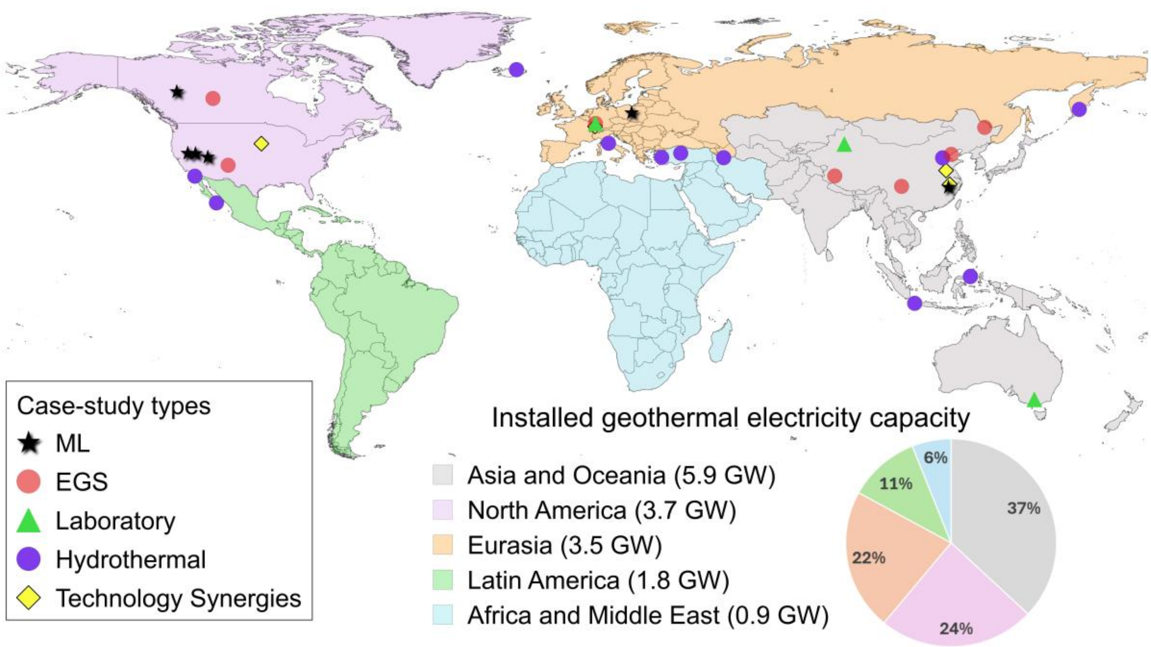

Fig. 14. Map of case studies described in the papers included in this scoping review and installed geothermal electricity capacity by region (modified from IRENA and IGA, 2023).

Negrín (2024) reviewed the evolution of the global geothermal industry for the 2020-2023 period and reported no change in Ethiopia's installed capacity since 2018 (7.3 MW).

The momentum in African geothermal development extends beyond Kenya and Ethiopia, with Eastern and Western states on the continent announcing exploration activities, thanks to investments projected to reach $35 billion by 2050 (AOW, 2024). Another country with promising development of its geothermal resources is Algeria, which is leading in the direct utilisation of geothermal energy in Africa. This has been supported by the government's energy efficiency and renewable energies program in 2011 (Lebbihiat *et al.*, 2021). In Algeria there is particular interest in electricity generation from medium enthalpy resources with ORC technology (Semmari *et al.*, 2024). Such growth would have Africa potentially surpassing Europe's geothermal capacity within the decade (AOW, 2024).

Latin America's geothermal potential is high thanks to the abundant volcano-hosted hydrothermal resources. However, only seven countries are producing geothermal electricity (Chile, Costa Rica, El Salvador, Guatemala, Honduras, Mexico, and Nicaragua). The industry leaders are Mexico, Costa Rica, and El Salvador, with 83% of the total installed capacity (1.7 GW) in the region (Castillo-Reyes *et al.*, 2024). In South America there is only one conventional geothermal power generation plant located in Cerro Pabellón (Chile) with an installed capacity of 80 MW (IRENA and IGA, 2023). According to Gutiérrez-Negrín (2024), Latin America showed an increase of 49.9 MW, a 3% increase over the period 2020-2023. This was mainly due to two countries: Chile, through the expansion by 33 MW of Cerro Pabellón, and Colombia, with 0.1 MW in a co-production plant. However, news and reporting on geothermal in South American countries seems to be increasing, as summarised in Table 5.

Figure 14 shows the installed geothermal electricity capacity was 15.8 GW in 2021. It also depicts the geolocations of the case studies described in the papers included in this review, and reported in Section 3.2. Worthy of note is the direct correlation between the regions with high installed geothermal capacity (Asia and Oceania, North America) and the number of numerical modelling investigations. The map also shows that North America is leading ML publications. Also of note is the diversity of projects in China where clearly EGS is of high interest. The northern hemisphere seems to be testing the possibilities of finding synergies between renewable technologies.

The lack of scientific journal publications in Latin America and Africa is a reflection of the developing status of these regions. As can be seen from the regional analysis above, industry expansion may be achieved through greater dissemination of the findings of simulation studies. Therefore, it is essential that research, academia and industry collaborate to assist these regions so that their geothermal potential can be realised. Financing and regulatory framework barriers to geothermal development in these regions are examined next. This is followed by a discussion on specific actions that governments, industry, and academia should take.

4.4.2. Barriers to geothermal development in South America and Africa

A geothermal industry can be developed in Africa and South America, but currently growth is still limited by high initial investment costs, technical complexity of geothermal exploration, unclear regulatory frameworks, social acceptance, and electrical grid integration (Castillo-Reyes *et al.*, 2024). Geothermal energy also has to compete with low-cost renewables, such as solar and wind (IRENA and IGA, 2023). The financing of these projects is hindered by these risks as well as by country-specific factors. These include investors' perceptions of local conditions such as social, political stability, market, unfavourable logistical and limited technical expertise. Mungai *et al.* (2022) identified barriers for investing in renewable energy in Sub-Saharan Africa, home to 14% of the world's population. Obstacles include reluctance of the private sector to finance projects to mitigate climate change; poorly executed or implemented policy and regulatory measures; and lack of state-based funding while subsidies of fossil fuel projects remain in place. The authors state governments and organizations should regard climate change as a development problem, rather than an environmental one.

To address some of the aforementioned risks and challenges, schemes such as the Geothermal Risk Mitigation Facility in the East African Rift (GRMF) and the Geothermal Development Facility in Latin America (GDF) have started to operate at a regional level (IRENA and IGA, 2023). Since 2012, for instance, the GRMF endorses early-stage development of geothermal projects in 12 countries (Burundi, Comoros, Congo, Djibouti, Eritrea, Ethiopia, Kenya, Rwanda, Somalia, Tanzania, Uganda and Zambia). Similarly, since 2016, the GDF Latin America has supported projects in 11 countries (Bolivia, Chile, Colombia, Ecuador, Peru, Costa Rica, El Salvador, Guatemala, Honduras, Nicaragua and Mexico). Financing mechanisms have also been offered by multilateral Banks (KfW, World, Inter American- and Caribbean- Development). The Japan International Cooperation Agency (JICA) has provided country-based risk mitigation solutions. This is offered by way of technical and financial assistance for geothermal project assessment and development.

The International Geoscience Programme (IGCPP), a flagship of the United Nations Educational, Scientific and Cultural Organization (UNESCO), supports the project called "Geothermal resources for energy transition". IGCP636 fosters international collaboration and young researchers' involvement in geothermal from 15 different countries. African and South American participant countries include Argelia, Chile, Colombia and Peru.

4.4.3. Policy Insights

Recently, the International Energy Agency (IEA, 2024) showed only 10% of the countries have active policies and/or regulatory framework on geothermal energy. Thus, the IGA is calling for awareness and education in this matter and understanding the terminology is relevant. Following Brommer (2025), *policies* are principles adopted by governments or institutions to achieve objectives as outlined in official documents. *Instruments* for policy implementation include regulations, financial incentives, market mechanisms, and voluntary agreements. *Primary legislations* are enacted by the parliament or congress to regulate sectors, including geothermal energy, environmental protection, and taxation. *Secondary regulations* are the rules established by legal authorities to manage specific activities. Subsequently, legislation and regulations form the structured set of procedural rules known as the *regulatory framework*. The latter in turn ensures compliance with laws and hence the policies.

In geothermal development the Act sets the legal framework while regulations define the procedures to be followed (Brommer, 2025). Policy implementation requires understanding how each country defines Acts and regulations. Costa Rica is one of the few countries that regulates geothermal under the environmental protection law. Kenya and Turkey take the mining law as a regulator. On the other hand, New Zealand and Iceland have a dedicated geothermal resources Act.

In summary, strong geothermal policies, and strong renewable energy targets are essential to achieving national targets to reduce CO_2 emissions, as shown in Figure 15. Costa Rica is the only Latin America country that seems to fit these criteria. Kenya, Chile and Canada seem to be on the rise but there is still room for improvement. Upcoming Congresses like LATAM (El Salvador, 2025) and World Geothermal (Canada, 2026) will provide good platforms to consolidate collaborative paths to move forward.

International policy recommendations focusing on reservoir simulations may contribute to the development of geothermal energy and should be embraced. A comparative and

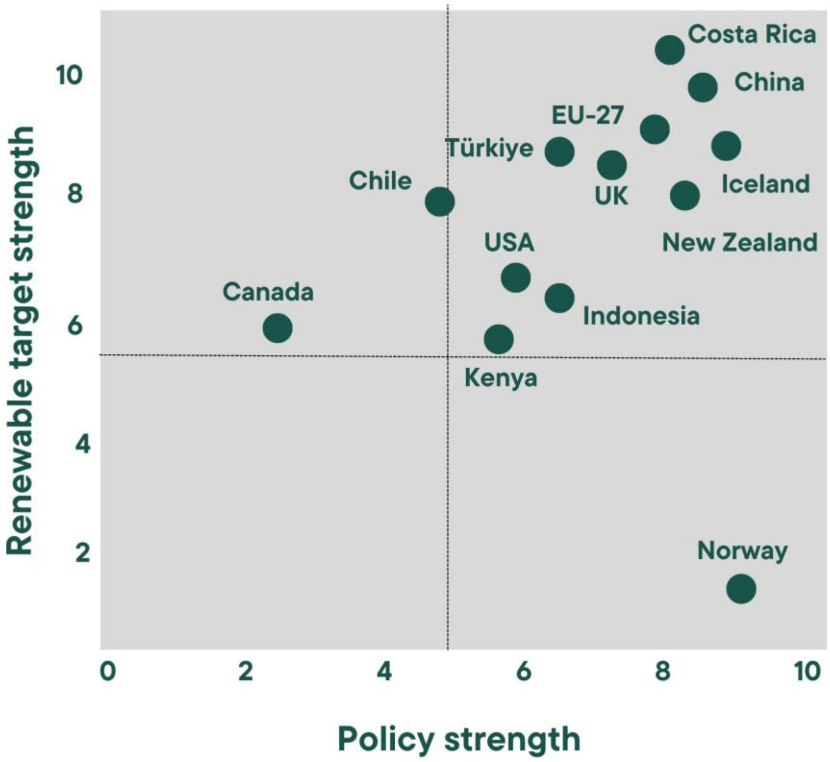

Fig. 15. Policy versus renewable target strength (Brommer, 2025), with permission of the author.

comprehensive analysis of current legal frameworks in the countries with identified geothermal resources should be conducted to identify how reservoir modelling is included. An exercise along these lines has been undertaken for South America by Torre Muñoz (2022). However, reservoir modelling was not discussed. As per O'Sullivan and O'Sullivan (2024) the benefits of carrying out computer modeling from early stages of a project have been widely demonstrated. This offers a valuable verification of the conceptual models and may assist in deciding the most critical data for understanding the system's behavior. Similarly, the guidelines for model calibration and validation required to ensure reliable and robust results by Nugraha *et al.* (2022) should be standardised worldwide.

Here we suggest items that should be included in new international policies focused on geothermal reservoir modelling:

1. Open-access database/collaborative platforms to promote sharing of available model inputs and results;
2. Government grants and programs to support research and development in advanced simulation technologies and methodologies;
3. Tax incentives (e.g., those based on CO_2 emissions) for companies adhering to geothermal simulation technologies;
4. Creation of advanced reservoir modelling training programs as per ESMAP (2023);
5. Inclusion of geothermal reservoir simulation topics in academic curricula in Earth Science-related schools and energy management courses.

4.4.4. Collaborative opportunities and industry development

Countries with established oil and gas industries, and geothermal potential have an advantage to pursue projects. Moreover, the interest for green hydrogen may represent an opportunity to expand geothermal development (IRENA and IGA, 2023). The application of geothermal direct uses based on heating and cooling needs is expected to take off, driven by dissemination, good practices and demonstration pilot projects, particularly in Chile and Central American countries (Aviña 2022; The World Bank 2023). Recently announced geothermal projects and research initiatives as listed below can also provide new collaborative opportunities and industry development:

1. The International Energy Agency Geothermal operates under the auspices of the Technology Collaboration Programme (TCP). Also called the Geothermal TCP, it fosters international collaboration to advance research, development, commercialisation and deployment. Its 6th term runs from 1 March 2023 to 29 February 2028. As of 2025 it has 16 members, none from Africa and only Mexico from Latin America.
2. The 12 Centers of Excellence in geothermal (CoEs) around the world, where cutting-edge research, international collaboration, and skill development are supported to address the challenges faced today in geothermal. The IGA's Academy fosters the relationships built with these CoEs (IGA, 2024).
3. The investment from JICA to develop the Chachimbiro project in Ecuador to build a 50 MW power plant (Project Management Global, 2024).
4. The startup Fervo Energy passed its 30-day well test. This milestone posts EGS as a promising and reliable technology that could be replicated worldwide (Golden, 2023).
5. The relaunch of geothermal energy in Italy, based on the discussion about the National Integrated Plan for Energy and Climate held between representatives of the government and experts from the industry and research institutions at the beginning of October 2024 (Cariaga, 2024).

4.4.5. Case study: Colombia

The promotion of this technology in countries along the Andean Mountain range with the use of reservoir simulation is crucial. Using Colombia as a case study, there are superficial exploration data from the 1980s. So far one exploratory geothermal borehole (Nereidas) was drilled in 1997 by the Nevado del Ruíz volcano (Monsalve *et al.*, 1998). The well, 1500 metres deep, registered a high bottomhole temperature (200°C), but no fluid. Because of the limited technical and financial resources available at that time, the subsurface exploration was stopped. González and Palacio (2021) reported this area has around 65 MW estimated power capacity. According to Alfaro *et al.* (2021), Colombia has 1.1 GWe untapped geothermal potential for electricity generation. This value needs to be validated with exploratory wells, given that high uncertainties affect the variables of the volumetric method applied for the estimation, since no measured subsoil data are available.

The Colombian geothermal licence requirements are now clear (Decree 1318, 2022; Resolution 40302). Decree 1598 of 2024, which modifies Decree 1073 of 2015, strives to introduce a competitive process for permit allocation, as well as providing guidelines to strengthen the interaction of developers with local communities. However, the implementation of these Decrees are time bound. Additionally, relevant financial incentives and risk mitigation mechanisms are needed, in particular for the drilling exploratory phase. The use of numerical modelling with ML enhancements should reduce uncertainties, and hence risks, including financial, involved in this phase of work.

Although in Colombia reservoir simulation is incipient (Vélez *et al.*, 2018; Moreno *et al.*, 2018), all parties involved in the field of geothermal energy would benefit from numerical modelling and/or ML at each stage of a project, i.e., exploration, prefeasibility, feasibility, development and production. This strategy could save modelling time and make it feasible for the country to start producing at least half of its current estimated potential in the next decade. Colombia could also gain time in its energy transition journey by producing geothermal energy through co-production with active oil wells, as the pilot projects described by Céspedes *et al.* (2022); to the use of depleted hydrocarbon wells; and abandoned mines.

4.5. Research and development opportunities

Another option that should be pursued so that tripling the size of the geothermal industry by 2030 (5 years from now) is achieved, involves scaling up production of developed projects. This needs to be done in parallel with outreach activities with local communities. This review shows there is room for investigation and improvement of numerical simulation through the use of ML in the modelling of four areas discussed below.

4.5.1. THMC processes

Several papers reviewed here dealt with THM or THC coupled processes, however, THMC (Thermo-Hydro-Mechanical-Chemical) processes were rarely addressed. According to Collard *et al.* (2023), surrogate geochemical modelling based on ML techniques has gained popularity in addressing the limitations of THM and chemical coupling. This is usually computationally expensive. An example is the use of ANN, XGBoost, or KNN for reactive transport modelling (Collard *et al.*, 2023). The understanding of THMC processes is critical to ensuring long-term sustainable and economically feasible geothermal field production.

4.5.2. Reinjection and induced seismicity

A sustainable field production also relies on a proper reinjection strategy, and locating the wells is probably the most important issue in the design step. This is an essential requirement for optimal geothermal field development, and can be addressed by numerical simulations (Rivera Díaz *et al.*, 2015; Kaya and Zarrouk 2017; Li *et al.*, 2023). Gerardi *et al.* (2023) provided a study of geomechanical numerical modelling of the Muara Laboh geothermal field (Indonesia), identifying the relationship between natural and induced seismicity and the activation of a fault zone due to reinjection. For seismicity risk management, robust and informative forecasting models must be developed (Ritz *et al.*, 2024). To face this challenge, ML techniques provide useful tools. One example is the unsupervised K-means clustering technique, shown in the work of Iaccarino *et al.* (2023) when analysing the moderate magnitude-induced earthquakes at The Geysers geothermal field in California.

4.5.3. Reservoir characterization

Another area that benefits from recent deployment of ML tools is reservoir characterization. In all types of geothermal resources, harnessed through conventional power technologies, EGS, or AGS, heterogeneity has a significant impact on fluid flow and heat transfer behaviour. ML can be used to explore subsurface uncertainty without the entire computational cost of numerical flow simulations to support optimum and timely decision-making (Maldonado-Cruz and Pyrcz 2022). The understanding of the physical mechanisms behind the engineering problem is very important for improve the performance of the ML tools to predict petrophysical parameters (Chen and Zhang 2020; Zou *et al.*, 2021; Maldonado-Cruz and Pyrcz 2022; Ali *et al.*, 2023; Castillo-Reyes *et al.*, 2023; Yan *et al.*, 2023).

It is useful to have methods that allow the inclusion of arbitrary discontinuities. However, modelling of the nonlinearity of fractured rocks remains a challenging area. Understanding of the effects of water cooling on fracture permeability enhancement and induced seismicity is also crucial, especially for EGS. More studies are needed on water mobility under supercritical conditions and its effects on thermal breakthrough.

4.5.4. Cross-industry and laboratory

Technology synergies of geothermal with other industries have been mentioned by the Department of Energy (DOE) since 2019. Promising applications for geothermal are direct use, thermal storage, clean heat for industry, and mineral recovery (DOE, 2019). Several possibilities for further reservoir simulation research to continue fostering innovation, driving collaboration, and accelerating growth in both the geothermal and related technologies are proposed here:

a) Modelling of scaling associated with critical mineral extraction from geothermal brines. A review by Szanyi *et al.* (2023) who also conducted a cost–benefit analysis to assess the financial feasibility of the technology could be used for reference.
b) The Stillwater triple hybrid power plant (Zhu and Turchi, 2017) and the recent conversion of the Alaşehir field where the geothermal power plant is being supplemented with solar, sets a worldwide example. The National Renewable Energy Laboratory's System Advisor Model (SAM), mainly used for techno-economic analysis of energy technologies, allows simulating of geothermal production and solar processes. SAM however, only considers the surface plant operation and does not allow subsurface simulation. This could open options for building a hybrid geothermal/solar simulator.
c) Silica from geothermal brines could be reused in CCS for CO_2 leakage containment (Castañeda-Herrera *et al.*, 2018) or to create an in-depth flow diverter (Llanos *et al.*, 2022).
d) The conversion of underground coal mines into geothermal resources has been considered in China since the beginning of this century, but most projects remain at the planning stage (Huang *et al.*, 2023). These authors analysed the feasibility and sustainability of harnessing energy from underground coal mines for heating purposes, through modelling with OpenGeoSys. The same software was used by Todd *et al.* (2024) in the context of underground thermal heat storage (UTES): THM modelling was conducted to analyse mechanical stability of the mine's structure during heat extraction and injection into the mine water systems. However, UTES resources are still under-utilised and heterogeneously developed across the globe (Goetzl *et al.*, 2023).
e) Experiments taking place at Monash University provide an excellent base for building numerical models to allow upscaling to field conditions. In the geothermal reservoir area this Australian group is researching three promising novel stimulation technologies for application in EGS and CCS, as follows:
   - *Foam based*, which requires minimum water and chemicals (Zhu *et al.*, 2020)
   - *Thermal*, with can generate complex microfractures (Harshini *et al.*, 2024)
   - *Slow releasing energy material*, an alternative to conventional techniques to control fracture propagation (De Silva *et al.*, 2018).

4.6. Strengths and limitations of this study

This study has identified the most frequently used simulators, under the constraints applied, and their contribution to the development of the geothermal industry. The discrepancy with the findings of O'Sullivan (2001) on most popular software is due to the timeframe and the basis of our scoping review being a database as opposed to the worldwide survey of all geothermal projects undertaken by O'Sullivan (2001). The inclusion in this work of emergent ML work opens the possibilities for new research projects. Additionally, the information relating to journals dealing with geothermal topics represents a useful guide for anyone interested in the study or application of geothermal reservoir engineering. However, this study has some limitations, as described next.

4.6.1. Boolean syntax

Elsevier's Scopus Application Programming Interfaces supports a Boolean syntax, i.e. a search that allows users to combine keywords with operators such as AND, NOT and OR to refine the search results. The operator AND was solely used for this review, which retrieved only those documents that, in the abstract, keywords and title, contained all the search terms. This limitation meant some published software-related papers might not have been identified in the search, for example, papers by Aguilar-Ojeda *et al.* (2021b) and Rinaldi *et al.* (2022) that dealt with TOUGH3. The former presents a MATLAB code for converting a three-dimensional conceptual model of Los

Humeros geothermal field (Mexico) from ArcMap to TOUGH3. The latter relates to CCS and nuclear waste disposal; however, the proposed approach has potential applicability for geothermal.

Based on ML papers included in this review, it was possible to identify that some publications used the term "system" instead of "reservoir" to define the geothermal subsurface complex. This means more manuscripts could have been identified using the operator OR ("reservoir" OR "system"). Additionally, a few papers in languages other than English, satisfied the Boolean search criteria (journals and years): for example, two TOUGH2 and ten COMSOL papers written in Chinese were identified. Also, the name of two simulators, STAR and STARS, required a specialised search term to differentiate them.

4.6.2. Other simulators and methodologies

The exclusion criterion used for this review implied discarding a paper by Croucher *et al.* (2020), because the main purpose of the paper was to describe the development of a new simulator, Waiwera. The results of this program however were successfully compared to outcomes from TOUGH2, TOUGH3 and AUTOUGH2. Waiwera was built at Auckland University, by the developers of AUTOUGH2 with the purpose of speeding up geothermal model runs. Hence, it is worth acknowledging the value of this new parallelised, object-oriented system written in Fortran 2003, as it is also the first to be released under a free, open-source software licence. Additionally, it is version-controlled using Git with developer documentation auto-generated using FORD1 and user documentation created using Sphinx. The up to sixty times faster simulation times achieved by Waiwera allow a faster calibration and refinement of models. These changes improve production predictions, support decision-making, and enable modelling to strengthen the value of geothermal projects. A few new geothermal simulators developed on the same methodology as TOUGH2 and comprise TOUGH+ (TOUGH2.2 rewritten in modern Fortran) and TOUGH3 (updated version of TOUGH2). Another promising software within the group of newest geothermal programs is Volsung. This simulator is combined with a graphical user interface and integrates reservoir., well and surface network models.

Potential contributions of well established codes using more modern programming languages and more integrated parallelization include OpenFOAM, OpenGeoSys, DuMux, PFLOTRAN, STOMP, FALCON (built on the MOOSE framework) and DARTS. An example of a novel application involves using PFC for studying the possibility of harnessing thermal energy from road pavement constructed using demolition waste in Australia (Baghban *et al.*, 2021).

Compared with analytical and experimental methods, numerical simulation can consider both complex boundary conditions and large-scale models with less investigation and a shorter calculation period. Finally, due to the use of the exclusion criterion, ML-related papers discussing the prediction of petrophysical parameters of subsurface reservoirs were not included (e.g., Chen and Zhang 2020; Zou *et al.*, 2021; Maldonado-Cruz and Pyrcz 2022; Ali *et al.*, 2023; Castillo-Reyes *et al.*, 2023; Yan *et al.*, 2023). However, these methodologies could be applied to geothermal reservoirs as discussed in Section 3.3.

5.Conclusions

The main motivation of the work presented in this article is to show how numerical modelling could assist in achieving the COP28 commitment. From 555 initially identified publications, 61 journal papers here included have allowed the screening of various modelling options to improve the understanding and performance of geothermal reservoirs. TOUGH2 is mainly applied for hydrothermal while COMSOL is used for EGS. The results also showed that North America is leading in the publication of ML case studies; China has high interest in EGS; while the northern hemisphere, particularly Europe, is researching synergies with renewable technologies. No case studies were reported from South America or Africa. Using structural, thermal, geophysical and geochemical archived data sets, ML is shown as a promising tool to assist in appraising developing geothermal fields. Additionally, technology synergy options could help maximise production in countries with mature geothermal industries. Such an integrated approach can accelerate the growth of the geothermal industry, and by fostering these strategies, economic, environmental, and social benefits can be achieved. More informed decision-making and reduced risks and uncertainties associated with geothermal reservoir development are also an additional benefit of a wider use of proper geothermal modelling tools. There is an intimate connection between simulation tools, optimum reservoir management, and field optimization.

Other challenges include improved accuracy in the simulation of heat transfer; fluid flow; mechanical aspects and chemical reactions simultaneously; and interactively. This multiphysics modelling approach should yield more cost-competitive utilisation of the geothermal resources. Addressing skill shortage is demanding, but regions and countries with suitable geothermal resources and existing oil and gas industries are in the best position to play to these natural advantages.

Tripling the output of geothermal energy by 2030 is a big task. However, attaining the target is feasible should numerical modelling be used from the exploratory project stages to abide more accurate decision making and lower overall project risk.

Acknowledgement: This work was conducted in the context of the IGCP636 Project "Geothermal resources for energy transition", supported by the International Geoscience Programme of UNESCO.

CRediT author statement: Both authors were equally responsible for the conceptualization, methodology, formal analysis, investigation, data curation and writing (original draft, review and editing).

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