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# Faradaic deionization technology: Insights from bibliometric, data mining and machine learning approaches

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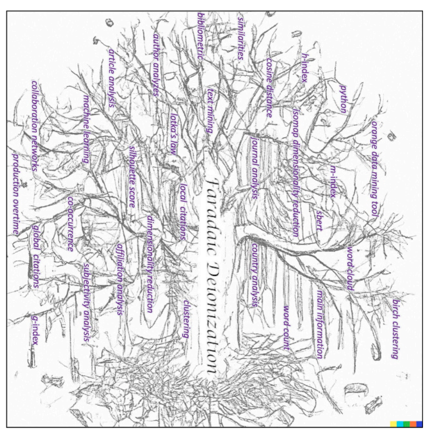
## HIGHLIGHTS

- Faradaic Deionization (FDI) dataset includes 170 papers downloaded from Scopus.
- Annual growth rate of FDI research based on published articles is 55.12 %.
- *Desalination*, *J. Mat. Chem.* and *ACS Appl. Mater. Inter*. are the core sources of FDI.
- China and the USA are the most active countries on FDI research.
- *Deionization*, *capacitive* and *desalination* are frequent words in FDI articles titles.

## GRAPHICAL ABSTRACT




## ARTICLE INFO

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## ABSTRACT

Faradaic deionization (FDI) is an emerging water treatment technology based on electrodes able to remove ionic species from water by charge transfer reactions. It is a young and promising technology that has attracted much attention due to its large capacity to store ions and the high selectivity of the faradaic electrode materials. This study reviews published papers on FDI from different angles: data mining, bibliometric and machine learning. Metrics such as annual growth rate, most important journals, relevant authors, collaborations maps, sentiment and subjectivity analysis, similarity and clustering analysis were performed. The results indicated that the strong interest in FDI really started in 2016, China is the most active country in FDI, and Desalination is the most important journal publishing FDI articles. The word cloud method showed that the most preferred adopted words are deionization, capacitive, electrode, material. Sentiment analysis results indicated that most of the researchers

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are optimistic about FDI technology. The title similarity method revealed that FDI researchers were successful in proposing unique and appropriate titles. The clustering approach stressed that FDI literature is concentrated on electrode material production, desalination application, lithium recovery and comparison with CDI.

## 1. Introduction

Depletion of natural freshwater sources makes low-cost, more sustainable, and high efficiency desalination systems a global priority. The worldwide installed seawater and brackish water desalination capacity has been increasing at a rate of ~40 % per year in the last decade due to global changes associated with population growth, aquifer shrinkage, industrial utilization or simply due to the COVID-19 pandemic [1]. This increase in worldwide installed desalination capacity (>100 million $m^3$ day by 2020) has been driven mainly by reverse osmosis (RO) technology, although multi-stage flash (MSF) and multiple-effect distillation (MED) technologies have been also adopted [2]. Electrochemical desalination systems, which include electrodialysis (ED) and capacitive deionization (CDI), are also viable technologies that have been mainly oriented to high water recovery and brackish water desalination, respectively [1]. CDI involves the application of an external electrostatic field (<1.5 V) between a pair of porous electrodes to induce the movement of ions towards the surfaces of the oppositely charged electrodes [3–8]. Specifically, ions are stored in the electrical double layer (EDL) formed between the solution and the electrode, which technically opens the possibility to store energy while treating water [7,9–16]. The core of the CDI technology are the pair of electrodes, and more precisely the active based materials. An intensive academic activity has been devoted during last 15 years to study different types of materials [17–20], mainly carbonaceous such as, activated carbons [21,22], carbon nanotubes [23–26], carbon aerogels [5,27,28], carbon fibers/cloth [29,30], carbon and graphite felts [31–34], graphene [19], polymer derived carbons [35–39], and composites [40,41]. In addition, a significant number of studies have been focused on biowaste precursors [42–49], activation mechanisms [48,50,51], heteroatoms doping [52–54] and metal oxide coated materials [28,55–58]. As an evolution of CDI systems, ion exchange membranes (IEMs) were incorporated to the CDI modules, giving rise to the known membrane capacitive deionization (MCDI) technology, whose main objective is to reduce the co-ion effect [59–62]. Furthermore, flow electrode capacitive deionization equipped with carbon suspensions was also introduced as a way of allowing continuous operation [63–66]. More recently, the focus, in terms of applications, have been shifted from desalination towards the use of CDI for wastewater treatment [10,67,68], and selective/preferential removal of certain ions or pollutants [69–73]. In this sense, the use of porous carbons in CDI systems revealed significant separation factors, specially between monovalent and divalent cations [74–76]. Thus, carbons with certain physicochemical properties can provide highly versatile ion-selective separations, due to different separation mechanisms [76], including those leveraging valence-based selectivity [77], size-based selectivity [78–80], and time dependent selectivity [81], among others. On the other hand, the use of customized IEM's enabled to achieve selective or preferential ion removal as well [76]. Thus, CDI and MCDI applications such as heavy metals removal [82–85], water softening [43,69,86], organic pollutants removal [67,69,87], nutrients capture [69,79,88–92], and resource recovery [76,93,94] have gained a remarkable visibility. Despite all these studies, only few pilot CDI devices are currently available in the market such as the ones provided by Voltea B.V. (The Netherlands/USA), ElectraMet (USA), Stockholm Water Technology AB (Sweden), Logicwater (India), EST Water & Technologies (China) and Siontech (South Korea). The reduced number of companies working in this research field evidences that more studies focused on treating real effluents are required to define the appropriate niche for CDI and to support the industrial implementation of this technology.

Like any other separation process, CDI technology also shows some drawbacks associated to: i) the limited desalination capacity (i.e. in most of cases, the salt adsorption capacity, SAC, lies below 30 mg $g^{-1}$ [95,96]), which is negatively impacted by the co-ion effect, although this is partially solved by MCDI thanks to the long-term stability of IEMs [8,97–100]; ii) the occurrence of side reactions, that affects to the oxidation of the positive electrode reducing the performance in the long-term, and iii) the discontinuous operation due to the two-step mechanism, which was solved by using flow electrodes performing the discharge step outside of the electrochemical cell [101].

To overcome these constraints, the scientific community was inspired by the developments achieved in the field of electrochemical energy storage, and more precisely, in material engineering for the fabrication of batteries [102–106]. The main difference between capacitive and battery materials is that faradaic materials employed in batteries store ions by means of faradaic reactions rather than using the ion electro-sorption in the EDL [104]. Thus, since faradaic reactions take place within the bulk of electrodes instead of just at the surface as it occurs when using capacitive carbon materials in CDI, higher desalination capacities were achieved by charge-transfer materials [95]. Moreover, faradaic materials avoid co-ion expulsion, which is one of the most significant disadvantages of CDI since it reduces the charge efficiency of the process [105]. Therefore, by using faradaic materials an important reduction of the energy consumption of the process can be achieved [102,104,107].

Attracted by the use of charge-transfer materials, a new stage of research began within the CDI community by exploring different material chemistries and configurations [8,106,108]. Two pioneer works should be highlighted in this case. First, Blair, et al. [109] in 1960 paired a chemically modified carbon electrode with Ag/AgCl for electrochemical deionization. Their main interest was focused on studying the effect of different modifications on the ion electro-sorption response of the carbon electrodes. This was the first study pairing a "non-carbon-based anion responsive electrode, silver-silver chloride" with a carbon-based electrode in an electrochemical system for water desalination. This combination of a charge-transfer electrode and a capacitive electrode was later defined as "hybrid capacitive deionization (HCDI)". In 2012, Pasta and collaborators introduced "A Desalination Battery" showing the evolution of the hybrid system into a full faradaic system [110]. An innovative system integrated by an electrode prepared from an intercalation material (a $Na_{2-x}Mn_5O_{10}$ nanorod, NMO) and an Ag/AgCl electrode was tested for seawater desalination. The desalination battery was able to store sodium ions within the NMO particles/layers by intercalation while the chloride ions were removed by a conversion reaction. This study represented the beginning of an emerging research line named Faradaic Deionization (FDI) in which charge-transfer materials, most of them previously tested for energy storage applications, were adapted to be used for environmental applications [93,102,106,108,111].

Initially, the selected materials were mainly oriented for $Na^+$ ions removal, since this cation is predominant in natural saline waters and water desalination was identified as one of the primary applications of FDI [93,95,112]. Among the commonly used materials, transition metal oxides (e.g. NMO [103,112,113], vanadium pentoxide [114,115], sodium titanium oxides [116,117], even binary metal oxides [118]), transition-metal hexacyanoferrates, also known as Prussian Blue Analogs (PBA's) [119–121], polyanionic phosphates (e.g. sodium iron phosphate, sodium phosphate titanium, sodium vanadium phosphates) [122], transition metal dichalcogenides (TMD's) [104,111,123], MXenes (e.g. two dimensional metal carbides, carbonitrides and nitrides) [124,125] and redox active polymers (e.g. polypyrrole, PEDOT; polyaniline, PANI; or naphthalene-polyimide PNDIE) [126–129] have been investigated. Regarding the anion removal, three different options were explored, i) to use a non-selective capacitive material, employing in this case HCDI modules [112,130–132], ii) to introduce an anion exchange membrane (AEM) by assembling a symmetric system composed by the oxidized and reduced form of the same electrode material. In this configuration the cell operates in a rocking chair mechanism in which the deficit of charge produced by intercalation/deintercalation of the cation is compensated by the anions crossing from one compartment to the other through the AEM [133]; iii) As a third option it was also proposed to use anion selective electrode materials such as Ag/AgCl [134], Bi/BiOCl [134] or polymers [135] in combination with cation removal electrodes, following the initial asymmetric faradaic configuration introduced by Pasta et al., in 2012 [110]. More innovative configurations involved the use of redox electrolytes instead of solid electrodes [136,137], the introduction of photoelectrodes [138,139] or the use of redox mediators [140,141].

Regarding the possible fields of applications of this technology, FDI was initially oriented to water desalination although further studies demonstrated its high potential for solving other critical environmental issues. The capacity of charge-transfer materials to perform selective/preferential electrochemical separations has expanded the FDI applications to pollutants removal [142–144], critical raw materials recovery [145,146] and recycling of battery compounds such as lithium-ions [102].

Despite the intensive work developed in the last decade in the proposed topic, many of the reported studies in the literature were developed at the laboratory scale and only few described pilot-scale FDI systems [147,148]. This is a faithful indication that FDI cells are still immature to meet the established requirements for commercialization. This can be attributed to some issues related with the stability of the charge transfer material at low concentrations, the cost of the cells (e.g., some configurations include the use of membranes increasing therefore the cell cost) or the lack of information and research studies on FDI using real effluents. To overcome these challenges and enable research and development, not only experimental tools should be developed and improved, but also theoretical models and computational approaches should be proposed because these have shown a huge potential in analyzing significant amounts of data with the aim of identifying specific patterns and trends.

A well-known technique for obtaining a statistical summary of a given field of interest is bibliometric analysis. Intellectual frameworks, distinctive research subjects and procedures, knowledge about authors, geographic locations of research institutions, and topic maturity can be assessed using bibliometric tools [149,150]. Last two decades have seen a significant expansion of bibliometric studies in different fields [151]. The bibliometric analysis includes mostly visualization of authors, articles, and journals with exploratory data analysis (EDA) and machine learning (ML) approach [152]. In this sense, the most widely used software for scientometric analysis is the Biblioshiny tool, which is part of the Bibliometrix package in R programming language developed by Massimo Aria and Corrado Cuccurullo [153]. In fact, Biblioshiny provides a complete set of tools necessary for science mapping workflow to conduct a thorough bibliometric analysis.

Briefly, ML is a promising area of computer science that attempts to predict outcomes by extracting patterns from massive datasets, generally in the form of a script that imparts extended knowledge of systems to detect and classify cases, and to identify patterns in unformatted or formatted datasets [154,155]. ML is divided into three basic categories: i) supervised learning, ii)- unsupervised learning, and iii)- reinforcement learning. Their applications vary from temporal dynamic vehicle-to-vehicle interactions to forecasting [156–158]. Moreover, Aytaç and Khayet [159] used an ML architecture to create the basis of the graphical abstract of their article. The unsupervised learning methods draw patterns from unlabeled data without considering established semantic relationships, making them appropriate for use with diverse data types like text, picture, audio, and video. By using data features, unsupervised learning techniques select what is meaningful in each domain [160]. This unsupervised learning is primarily used for dimensionality reduction, density estimation, clustering, and anomaly monitoring [161,162]. Dimension reduction (DR) techniques are considered to decrease the number of input features in a given set of data, rendering it more compact to improve the learning algorithm's efficiency [163]. DR can help users to reduce the data storage space, to decrease the computational time of ML algorithms, and to help visualizing multidimensional data in lower dimensions such as 2D or 3D [164,165]. Clustering is a sub-branch of unsupervised learning methods, basically partitioning a dataset into segments so that data points within a cluster become similar to each other although data points across sets differ [166]. Clustering algorithms are used in many ways to obtain insight into the data structure [167].

The process of finding and extracting implicit, undiscovered, and potentially useful information from a large-scale text collection using ML, Natural Language Processing (NLP) and statistics is known as text mining (TM). The use of text mining methods to identify patterns and gaps, and indicate important future trends is extremely helpful for the studied domain [168,169]. Textual data can be used for finding the percentage of words naturally referring to topics (clustering), counting particular words (word cloud approach), finding data similarities in specific cases (similarity analysis), and reflecting opinions (sentiment and subjectivity analyzes) [170]. TM approaches include various steps to identify valuable information from the meta-data. The first one termed text preprocessing involves cleaning up the text by removing stop words, tokenization, stemming, lemmatization, and vectorization among others; and converting it into a format that computers can use. Preprocessing textual data for a certain topic is essential for analysis, finding correlations, and other useful tasks [171,172]. Tokenization is a method of breaking down, dividing, and converting a corpus into alphabets or words [173]. Stemming step, which aims to group all variations of a word into one group and lemmatization, which is the process of computing canonical forms of words in a text, are two very important preprocessing stages to aid Natural Language Processing [159]. Vectorization is a process of converting unstructured data to a computable form. The bag-of-words (BoW) approach, which counts how frequently each word appears in each item is utilized mostly [174]. Word clouds are a visual way to portray textual data that emphasize frequency and clearly defined groupings of items. By highlighting terms that commonly appear in each set of corpora, this kind of visualization can help assessors with exploratory textual analysis. Additionally, this method may convey the most important ideas or themes throughout the reporting phase [175,176]. TM techniques are crucial in tasks such as finding similar patterns, summarizing, searching, or classifying, as well as machine translation [177,178]. Sentiment analysis is for understanding people's views and opinions based on text data. Likewise, subjectivity analysis is important in revealing the level of subjectivity or objectivity of a corpus, and this type of analysis is widely addressed in NLP [179,180].

In this paper, we reveal the trends and patterns in FDI literature by bibliometric, data mining, and machine learning methods. The Biblioshiny tool (Bibliometrix package) in R programming language is used to disclose the bibliometric trends. Python and Orange Data Mining Tool were used for ML, and TM approaches.

## 2. Data and methodology

### 2.1. Data

The dataset required for this research was obtained on September 30, 2022, from the Scopus database. Our research criteria for publication year started from 2012, when the first FDI article was published, up to the year we downloaded the data set. We did not include the

**Table 1**
Search criteria for FDI articles and reviews.

| Criteria | Description |
|---|---|
| Title-Abstract-Keyword | ***Limit to*** Keyword List (Table 2) |
| Source type | ***Limit to*** Journal |
| Document type | ***Limit to*** Article ***OR*** Review |
| Publication stage | ***Limit to*** Final |
| Language | ***Limit to*** English |
| Publication year | ***Limit to*** from 2012 to 2021 |
| Subject area | ***Limit to*** Engineering ***OR*** Chemical Engineering ***OR*** Environmental Science ***OR*** Chemistry ***OR*** Energy ***OR*** Material Science |

publications of the year 2022 to be able to compare the yearly published articles. The Scopus database was chosen because it covers publications that meet a stringent set of requirements, and its scientometric information for publications indexes is complete. Furthermore, the Scopus database is better suited for mapping new areas of research that may not be adequately represented by other databases such as FDI [181,182]. The followed search criteria can be seen in Table 1.

For the present study we used a large keyword repository to cover all publications the domain might contain. The list of keywords we have considered, and the raw numbers of results are given in Table 2.

In the next stage of the study, we reduced the dataset by first deleting the duplicates and then screening the collection to remove unrelated articles. The final dataset contained 170 publications.

### 2.2. Methodology

The Biblioshiny tool in Bibliometrix library using R Programming Language was employed for bibliometric analysis. The basic statistical calculations used by Biblioshiny are as follows.

$$\text{Average citations per article published in the corresponding year} = \frac{TC_n}{(Y_f - Y_n) \times ND_n} \tag{1}$$

where $ND_n$ is the number of articles in the year $n$, $Y_f$ is the final year of publications in the collection, $Y_n$ is the publication year of the articles and $TC_n$ is the total citations of the articles in the year $n$ [183].

$$(Compound)Annual\ growth\ rate\ (\%) = \left(\left(\frac{ND_f}{ND_i}\right)^{\frac{1}{(Y_f - Y_i)}} - 1\right) \times 100 \tag{2}$$

where $ND_f$ is the number of articles of the final year, $ND_i$ is the number of articles of the initial year, and $Y_i$ is the initial year of the publications in the collection [184].

$$International\ Co\text{-}Authorship = \frac{ND_{ca}}{ND} \tag{3}$$

where $ND_{ca}$ is the number of documents published by co-authors from different countries and $ND$ is the number of documents in the collection [185].

$$Co\text{-}Authors\ per\ document = \frac{NA}{ND} \tag{4}$$

where $NA$ is the author appearances [186];

$$\text{Document average age} = \frac{\sum_{i=1}^{n} DA_i}{ND} \tag{5}$$

where $DA_i$ is the age of the document.

$$\text{Average citation per document} = \frac{\sum_{i=1}^{n} DC_i}{ND} \tag{6}$$

where $DC_i$ is the citation number of the document.

$$Articles\ fractionalized = \sum_{i=1}^{m} \frac{1}{N_{ca}} \tag{7}$$

where $m$ is the number of co-authored documents of the author, and $N_{ca}$ is the number of co-authors [187].

The $h$-index is the highest number of articles of an author having at least $h$ citations [188]. The $g$-index is a unique value that shows the quality of a researcher or journal and indicates that at least $g^2$ citations were received by the top $g$ articles [189]. The $m$-index is a metric that shows the $h$-index per year value of an author/journal and can be calculated as follows.

$$m - index = \frac{h - index}{Ya_f - Ya_i} \tag{8}$$

where $Ya_f$ is the year of the final publication of the author and $Ya_i$ is the year of the initial publication of the author [190].

Global citations refer to the total number of cited by the value of an article (or researcher) in the collection of documents found in bibliographic databases (Web of Science, Scopus, etc.). As a result, the global citations track citations for a chosen article from all over the world. On the other hand, local citations refer to the number of times an author or a document in the collection has been cited by articles in the same collection [186,191].

Lotka's Law indicates the number of authors $(y_x)$ contributing with $x$

**Table 2**
Keyword list considered to collect FDI articles.

| Keyword | Number of papers |
|---|---|
| Prussian blue | 3531 |
| FDI | 2140 |
| Desalination performance | 824 |
| Redox polymers | 535 |
| Faradaic reactions | 508 |
| Reversible redox reactions | 416 |
| Intercalation mechanism | 411 |
| Brackish water desalination | 356 |
| Intercalation materials | 174 |
| Intercalation electrode | 162 |
| Faradaic electrodes | 77 |
| Hybrid capacitive deionization | 76 |
| HCDI | 62 |
| Desalination battery | 32 |
| Hybrid CDI | 27 |
| Faradaic electrode materials | 23 |
| Berlin green | 19 |
| Faradaic materials | 17 |
| DEDI | 15 |
| Faradaic deionization | 10 |
| Faradaic systems | 5 |
| Ion-intercalation processes | 3 |
| Dual-ions electrochemistry desalination device | 1 |
| Hybrid Faradaic capacitive deionization | 1 |
| Faradaic electrochemical deionization | 0 |
| Total | 9424 |

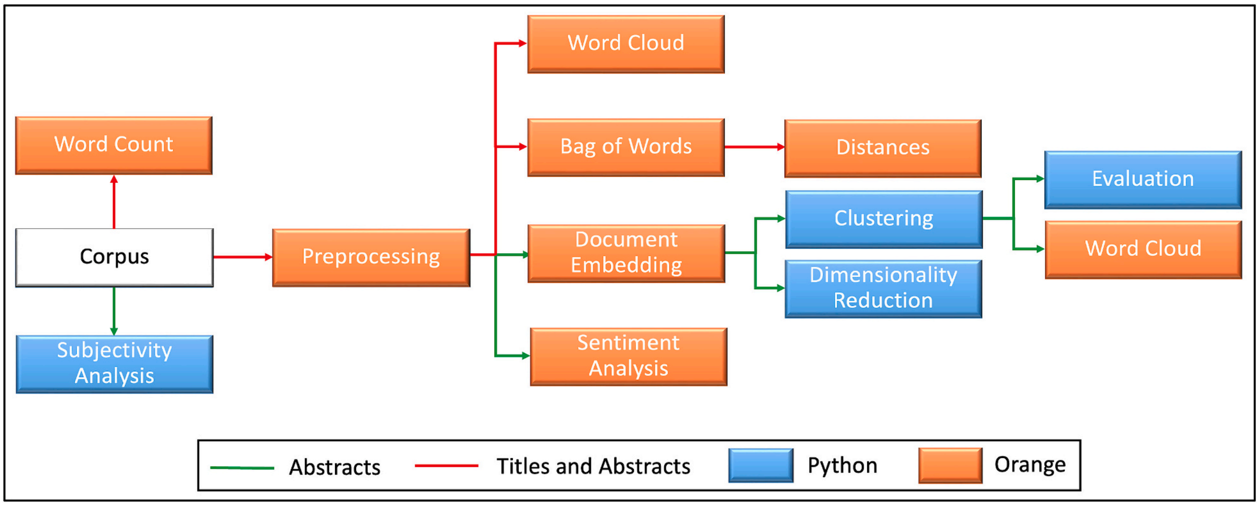


**Fig. 1.** Flow chart of the TM/ML process.

publications within the subject:

$$y_x = \frac{C}{x^a} \quad (9)$$

where $C$ and $a$ are two constants calculated in the domain and are close to $\frac{6}{\pi^2}$ and 2, respectively [192,193].

For TM and ML analysis Python and Orange Data Mining Tool were used. The basic process sequence can be seen in Fig. 1.

The preprocessing stage consisted of the transformation (converting to lowercase, converting accents), tokenization, filtering (removing stop words, lexicon, numbers, and regular expressions), and normalization (stemming and lemmatization) of the dataset. For the sentiment analysis, Orange uses Valence Aware Dictionary for Sentiment Reasoning (VADER) approach. Built on a dictionary that maps lexicons to emotion intensities, VADER refers to a sentiment score, which is calculated by adding the intensities of each item in the text. Then the compound sentiment score, which is the normalized summation of positive, negative, and neutral scores, is shown between −1 (most negative) and +1 (most positive) [186,194]. Subjectivity measures the degree of personal opinion and factual information in a text. This approach is used to categorize text as subjective (including an opinion) or objective (factual) [180]. In this case, the Textblob library in Python was used for subjectivity analysis being the subjectivity value between 0 (very objective) and 1 (very subjective) [195].

Bag-of-words (BoW) method was used to find similar titles/abstracts in the dataset. This is a basic yet efficient method of representing textual data using word frequency vectors. It transforms the document by using a method called term frequency ($tf$), which is based on frequencies of the words in a data instance. In this case, a data sample is represented by a vector where the frequency of a word is 1 if this word occurs among all words in the corpus and 0 if it does not [196]. The similarities were then calculated using cosine similarity (CS). The main idea in CS is to compute the cosine value of the angle between two vectors to show their similarity. Cosine similarity has a value between −1 and 1. In particular, the CS value is equal to −1 when two vectors are pointing in opposite directions and 1 when they are pointing in the same direction. The following equation (Eq. (10)) can be used to calculate CS for two vectors, $X^T = \{x_1, x_2, \ldots\ldots x_N\}$ (vector 1) and $Y^T = \{y_1, y_2, \ldots\ldots y_N\}$ (vector 2) [197];

$$CS\,(X, Y) = \frac{\sum_{i=1}^{N} x_i\, y_i}{\sum_{i=1}^{N} x_i^2\ \sum_{i}^{N} y_i^2} \quad (10)$$

Finally, the distances between each data instance were calculated using cosine distance (CD), which is $1 - CS$ [198]. The document embedding was applied using Sentence – BERT (SBERT) transformer-based language model. SBERT is a modification of the Bidirectional Encoder Representations from the Transformers deep learning model (BERT). SBERT is similar to BERT pre-trained transformer network, except it discards the final classification header and processes one sentence at a time. SBERT can then generate the embedding using average pooling in the final output layer. Unlike BERT, SBERT is trained on sentence pairs using a siamese architecture. Consider having two identical BERTs running in parallel with the same network weights. SBERT in Orange converts sentences or paragraphs into vectors of size 384. More details about SBERT architecture can be found elsewhere [199]. After embedding the abstracts, the dataset was clustered using Balanced Iterative Reducing and Clustering using the Hierarchies (BIRCH) algorithm. The BIRCH algorithm creates a hierarchical tree of the dataset where the number of clusters ($K$) is determined by the users. BIRCH algorithm finds the clusters by creating clustering feature ($CF$) tree $\left(CF = \left(N, \overrightarrow{LS}, SS\right)\right)$, where $N$ is the dimensions of data points, $\overrightarrow{LS}$ is the linear sum data points and $SS$ is the square sum of data points. $\overrightarrow{LS}$ and $SS$ can be calculated using Eqs. (11) and (12), respectively [200,201].

$$\overrightarrow{LS} = \sum_{i=1}^{N} \overrightarrow{X_i} \quad (11)$$

$$SS = \sum_{i=1}^{N} \left(\overrightarrow{X_i}\right)^2 \quad (12)$$

where $X$ is a data instance.

The cluster centroids $\left(\overrightarrow{C}\right)$ can then be determined as follows (Eq. (13)):

$$\overrightarrow{C} = \frac{\overrightarrow{LS}}{N} \quad (13)$$

The radius of the clusters ($R$) is calculated using the following equation (Eq. (14)):

$$R = \sqrt{\frac{SS}{N} - \left(\frac{\overrightarrow{LS}}{N}\right)^2} \quad (14)$$

The number of clusters ($K$) must be defined by the user, so a metric must be used to find the optimal $K$ value. The silhouette score is a useful statistical approach for evaluating or validating $K$. This metric considers each data point's distance from its cluster and surrounding clusters. A data's silhouette score $(s(i))$ may be determined as shown in the following equation:

$$s(i) = \begin{cases} 1 - \frac{b(i)}{w(i)} & if b(i) < w(i) \\ 0 & if b(i) = w(i) \text{ and } b(i) = \min_{K}\{B(iK)\} \\ \frac{w(i)}{b(i)} - 1 & if b(i) > w(i) \end{cases} \tag{15}$$

where $w(i)$ is the average distance between the $i^{th}$ point and the other points in its cluster, $B(i,K)$ is the average distance between the $i^{th}$ point and points in another cluster $K$.

By using the intra-cluster silhouette values of data points, the silhouette score of each cluster $(\underline{s}(K))$ can be determined as follows [202].

$$(\bar{s}(K)) = \frac{\sum_{i=1}^{n} s(i)}{n} \tag{16}$$

where $n$ is the number of data instances in the cluster.

The value of silhouette score ranges between $-1$ and 1. When it is close to $-1$, it indicates a poor clustering; but when it is about 1, it means a perfect clustering.

For the visualization of clusters in 3D space, a dimensionality reduction approach was employed by means of the Isometric Mapping (ISOMAP). This is a pairwise geodesic distance-based nonlinear unsupervised isometric mapping method. The geodesic distance measurement is the sum of edge weights along the shortest path between two nodes [203]. ISOMAP initially creates a neighborhood graph by calculating the geodesic distances between data, $x_a$, and its nearest neighbors. Then, the shortest path between each data instance in the neighborhood graph is calculated to approximate the geodesic distance between them, and a pairwise geodesic distance matrix $(d^G)$ is built. Subsequently, kernel matrix ($KM$) is calculated using Eq. (17):

$$KM = H\, d^G\, H \tag{17}$$

where $H$ is the centering matrix. The low dimension embedding of a data point ($Y$) is then calculated by ISOMAP (Eq. (18)).

$$Y = \widehat{D}^{1/2} B_1^T \tag{18}$$

where $\widehat{D}$ is the diagonal matrix of the top $k$ Eigenvalues and $B_1$ is the top $k$ Eigenvectors [204].

## 3. Results and discussions

### 3.1. FDI technology dataset

Through the visualization of information, scientometrics can effectively illustrate the direction of most of the research in a field. The first step of our bibliometric analysis was to present the main information about the collection to reflect the facts, which can be seen in Fig. 2.

Since FDI is a recently developed technology, it can be understood from the timespan that the published articles were very recent. This is also confirmed by the document's average age score (2.62). Although the number of FDI articles published is low (170), the high number of sources (61) is an indicator of how much interest and acceptance had been received for FDI by journals. The number of authors, which is 472, is moderate when considering the number of articles. The ability to analyze co-authorship patterns is made possible by the availability of author address meta-data on publication indices. Measures of scientific papers with two or more authors from different nations are known as international co-authorship. This is an interesting parameter to measure the collaboration of authors in the concerned domain [205–207]. The international co-authorship value (25.29 %) indicates that the internationality rate of this new technology is sufficient. The average citations per document (46.69) also informed that FDI received a good number of citations considering the short document average age value. The yearly FDI publications and the average citations per article published in the corresponding year can be seen in Fig. 3.

Although the FDI process did not receive enough attention for a short time after the publication of the first article in 2012, a continuous growing interest began 4 years later. This could be attributed to the more attractive properties of cheap and accessible carbon materials employed in CDI, a technology that was starting its exponential growth in terms of publications and citations at a time [208]. Looking at the timeline of the application of intercalating materials published by Singh, et al. [106] in 2019, one might realize that significant research studies regarding the use of materials (sodium iron phosphate [112], MXene [124] and PBA's [209]) and modeling [1] were published that year serving as a starting point of this renewed interest for the FDI technology. Because of the increment of publications, the average number of citations normalized per year started to decrease from its maximum (57.6) in 2015 to about 9.3 in 2021 (Fig. 3).

### 3.2. Authors of FDI articles

Presenting prominent authors in a particular field to readers is one of the cornerstones of bibliometric analysis. The evaluation of the FDI authors in quantitative and qualitative ways was carried out with exploratory data analysis. Fig. 4 shows the number of articles published

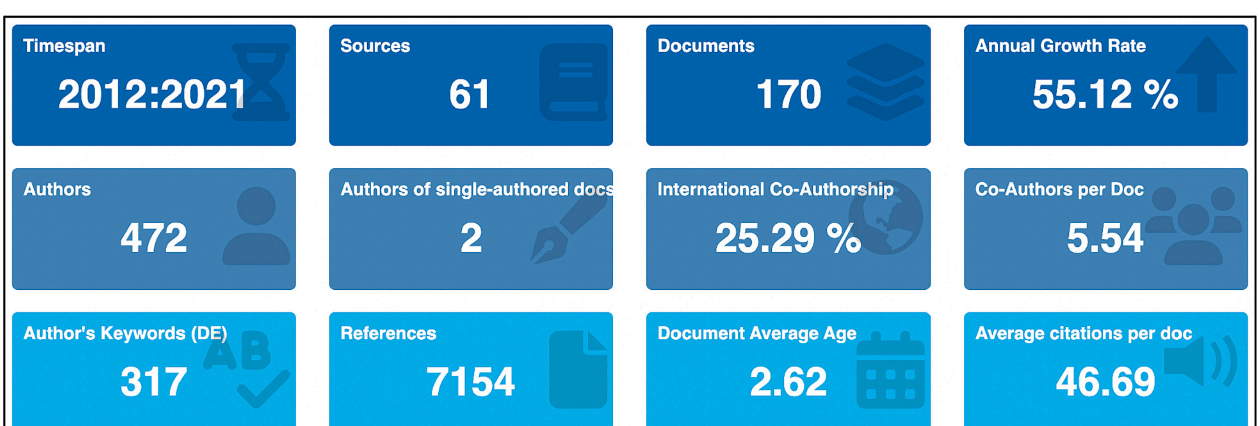


**Fig. 2.** Main information about the FDI domain.

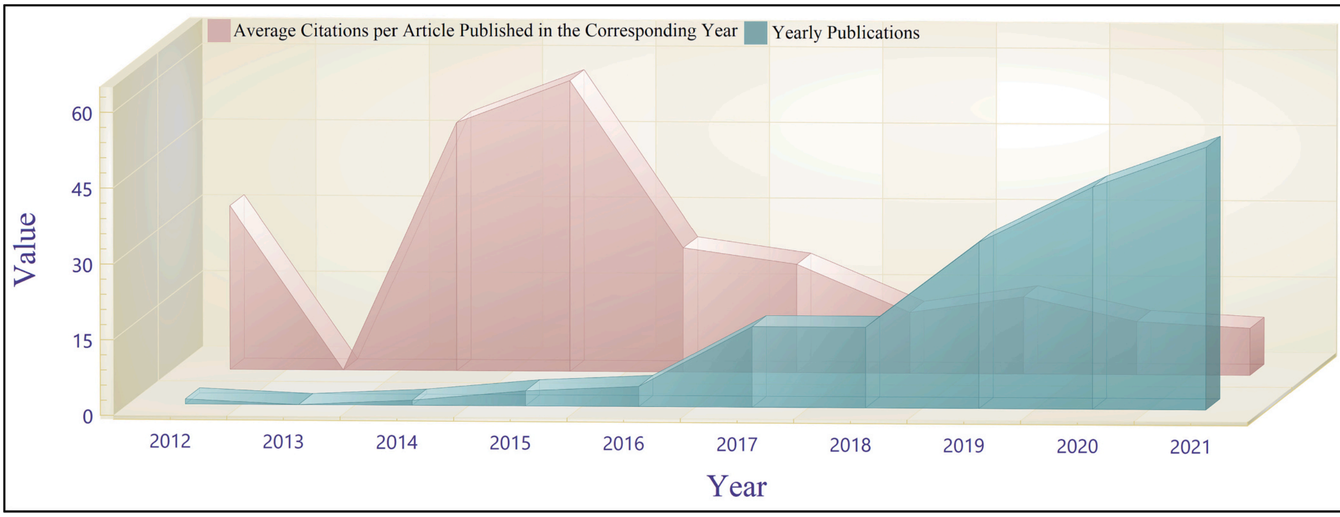


**Fig. 3.** Yearly FDI publications and the average citations per article published in the corresponding year.

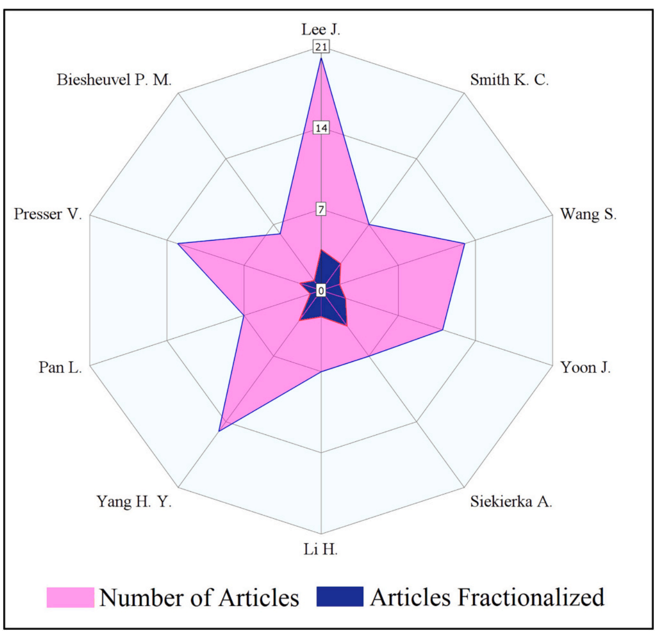


**Fig. 4.** Number of FDI publications and articles fractionalized of the top 10 authors (for each affiliation indicated in an article, only the author with the highest metric is linked to that article).

by the top 10 authors in the FDI field. To avoid counting an article multiple times, of each affiliation indicated in this article, only the author with the highest metric is linked to that article.

The fractionalized value in Fig. 4 measures each individual author's contribution to a collection of published articles. Lee J. affiliated to the Korean group in Seoul National University (SNU) published 20 papers. Among them, it should be highlighted that Lee and collaborators coined the term "HCDI" when they replaced a capacitive electrode by an NMO electrode, leading to a significant increase of the salt adsorption capacity from 13 mg $g^{-1}$ to 31 mg $g^{-1}$ [112]. Furthermore, Lee J. made significant contributions using novel electrode materials such as $Na_2FeP_2O_7$, NMO, $MnO_2$, PBA's or silver coated carbon composite materials not only for water desalination but also for lithium recovery [122,130,133,210,211]. On the other hand, Yang H. Y. performed most of her studies at Singapore University of Technology and Design (SUTD) where she published 15 articles about FDI until 2021. Among those studies, the results reported about an all-faradaic deionization system integrated by NMO and BiOCl electrodes that reached a SAC capacity of 68 mg $g^{-1}$ should be highlighted [212]. Other studies of special interest involved some other all-faradaic systems integrated by AgCl and NMO but also HCDI systems composed of PBA's and activated carbons [134,213].

Fig. 4 shows that the researcher with the highest articles fractionalized value is Siekierka A. (3.78). This value indicates that Siekierka A. published articles with very few co-authors in his research group. The bibliometric analysis indicated that both groups (SNU and SUTD) added a significant scientific production on FDI. Besides, when the fractionalized article values were examined, it was seen that that of Yang H. Y. (3.20) was close to that of Lee J. (3.51). When these values are compared, it is understood that Yang H. Y. produced publications with fewer co-authors than Lee J. The analysis of the production overtime, which shows the continuity of the published FDI articles by authors over the years and citation numbers, is one of the most discussed bibliometric methods. The production overtime as well as the global and local citations graph of the top 10 authors dedicated to FDI research is shown in Fig. 5.

Fig. 5(a) allows us to examine the authors who had a continuous dedication to FDI research. In this case, authors ́ production overtime includes only one author from each affiliation to avoid counting articles multiple times. As can be seen, Lee J., Kim C., Kim S, and Yoon J. are the longest-standing researchers in the FDI field, although Yoon J. is one step ahead of Lee J., Kim C. regarding article publishing continuity, since this author has published at least one paper annually. Jeyong Yoon is the leader of the Water Environment and Energy Lab of SNU (South Korea), who has been actively working on electrochemical technologies for environmental applications developing a very fruitful career. As commented before, he has extensively collaborated with Lee J. in electrochemical ion separation (EIONS) technologies and has participated on 6 review papers about the use of capacitive and charge-transfer materials for electrochemical water treatments [76,102,214–217]. In the case of Choonsoo Kim, he is the head of the Environmental Electrochemistry Lab in Kongju National University (South Korea) and has also been involved in a research collaboration with Yoon J. and Lee J. Kim, C. has also made significant contributions to the field, specially using the multichannel deionization system [216,218–220]. The multichannel desalination battery (MC-DB) introduced the idea of using a highly concentrated solution between the electrodes and the brackish water to be treated, just separated by ion exchange membranes. The role of this additional channel would be to overcome the intrinsic mass-transfer limitation at the electrode–electrolyte interface of the

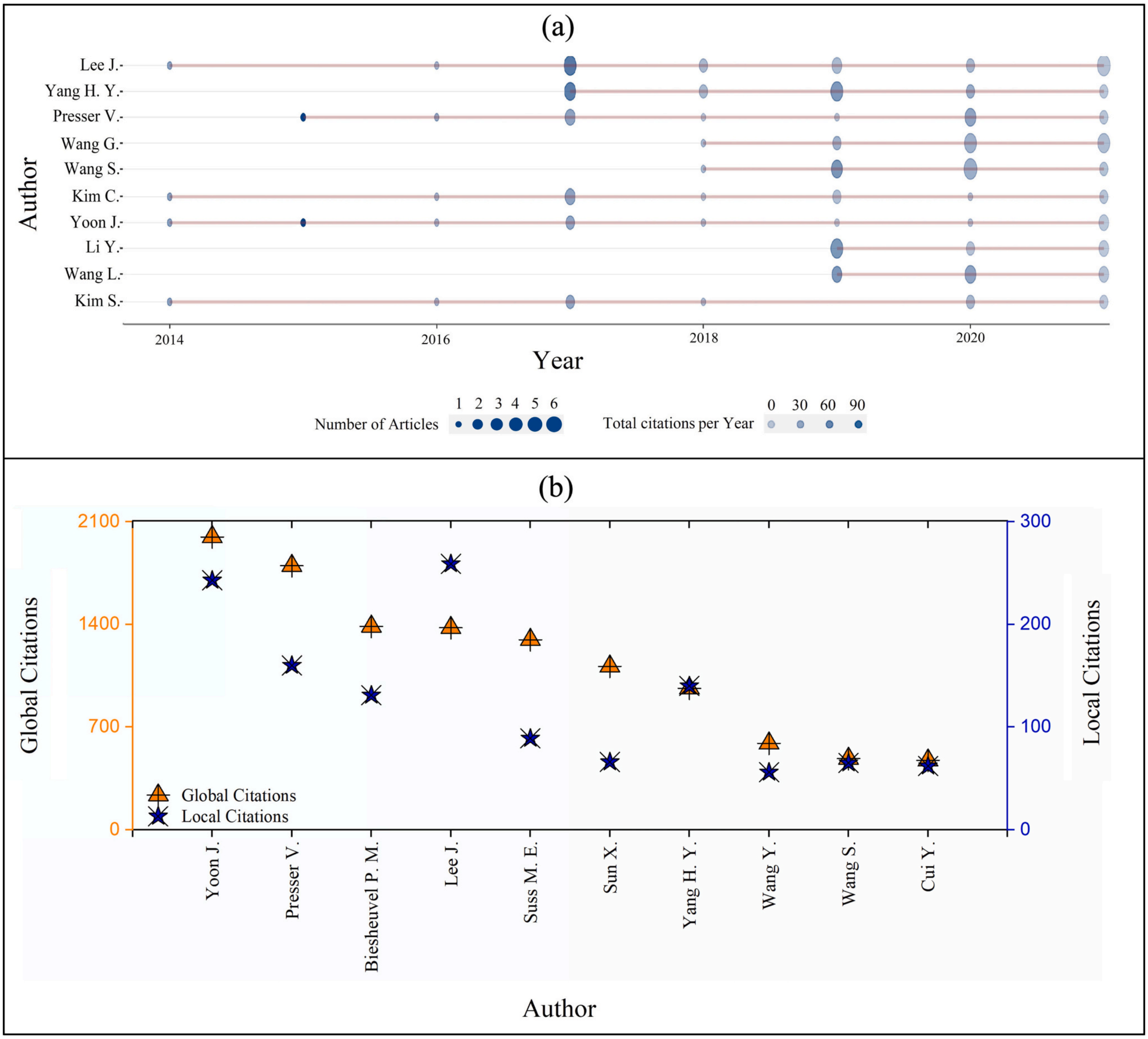


**Fig. 5.** (a) Production of the top 10 authors in FDI overtime. The graph includes the number of articles published in the field (size of the circle) and the total citation per year (color of the circle). (b) Global and local articles citations of the top 10 FDI authors. (For each affiliation indicated in an article, only the author with the highest metric is linked to that article).

desalination battery. The authors showed how the increase of the concentration of the side channel solution led to a relevant SAC improvement from 17.4 to 52.9 mg $g^{-1}$.

Considering that citations are a crucial sign of the quality and significance of a published work, the citation-based analysis offers an objective signal for authors' influence in each domain. In this case, Fig. 5 (b) shows the top 10 FDI authors based on the global and local citations of their articles. Note that just the author with the highest metric from each affiliation indicated in each article is displayed on Fig. 5(b). Considering the articles written about FDI, it has been revealed that up to the date the dataset was fetched, the most globally cited author is Yoon J. with 1996 citations followed by Presser V. and Biesheuvel P.M. with 1800 and 1386, respectively. Volker Presser is the leader of the program division “Energy Materials” at Leibniz Institute for New Materials (INM, Germany) and professor at Saarland University in Saarbrücken (Germany). In his group, researchers have explored and developed electroactive materials and interfaces for the energy/water nexus by hybridizing nanoscaled carbon interfaces with Faradaic materials. Presser V. has actively participated in the development of FDI technology by publishing high quality review articles (4) pointing out not only the state-of-art but also the challenges and opportunities [6,95,102,214]. Occupying the third position in the ranking of highly cited authors, Biesheuvel P.M. has contributed with valuable articles not only in the FDI field but also in the water treatment field. P. Maarten Biesheuvel is the coordinator of the Advanced water treatment at Wetsus research center (The Netherlands) and has a significant track record of valuable articles describing the theory and modeling of CDI and MCDI processes [6,59,214,221–223]. Regarding FDI, Biesheuvel and collaborators have reviewed recent advances on ion selectivity using charge transfer materials while exploring the use of PBA's for mono/divalent separations [76,119]. Since local citations measure the number of times a document/author in this collection is cited by documents in the collection, this metric is one of the most important indicators of how important a document is in the field of study. When we consider the local citations, in contrast to his global citations, Yoon J. was in the second position after Lee J. with citation values of 243 and 259, respectively.

As stated previously, to understand the productivity and impact of authors in the FDI domain, some authors' metrics like *g*, *h* and *m* have been evaluated. These indices point out the authors of a domain in a qualitative way. The obtained metrics of the top 10 authors in the collection based on *h*-index and the corresponding *g* and *m* indices can be seen in Fig. S1. While Lee J. is ahead in the *g*-index and *h*-index with values of 20 and 14, respectively; Wang S. is in the first position in the *m*-index with a value of 2.2. Shiyong Wang has dedicated his research at Dalian University of Technology (China) mainly to the preparation of innovative electrode materials (metal oxides, PBA's, NMO, MXenes) for CDI and HCDI [224–227].

As in any discipline, collaboration is essential for the advancement of science. Performing an analysis on authors' collaboration helps to find out the connections between scientists and know the main authors clusters in the field under study. In FDI bibliometric analysis, Fig. 6 illustrates the collaborations carried out between authors and the involved clusters and corresponding author's country.

Fig. 6(a) shows not only the connections of the authors in the FDI domain, but also the important collaboration clusters in the collection and the strength of these connections. The number of publications of an author increases with the node size, while the number of authors working together increases with the edge thickness. As can be seen in the figure, the collection pointed to 7 groups. The largest one, led by Lee J., is the purple cluster made up of 8 researchers. This cluster represents a strong collaboration between the Korean groups of Seoul National University (Lee J., Yoon J., and Kim S.), Kongju National University (Kim C.) and the German group (Presser V., Srimuk P., and Aslan M.). The second dominant cluster, headed by Yang H. Y., is the pink collaboration network formed by 6 researchers all from Singapore University of Technology and Design (SUTD). While Yang H.Y. had a smaller collaboration network in this topic, mainly restricted to SUTD, Lee J. had expanded his network among other institutions not only in South Korea but also internationally performing collaborations with Presser's group in Germany. The other two large clusters are composed by researchers from Dalian University of Technology, with Wang G. the most productive researcher, and East China Normal University with Linkun Pan as a leader of the group.

The corresponding author of an article is the researcher in charge of all types of communication with the editorial of the journal. This kind of analysis is a good criterion for measuring the scientific performance of countries and authors together. Fig. 6(b) illustrates the countries of the corresponding authors with the data of single or multiple country publications.

China ranks first in both single country publications number (53) and multiple country publication number (12). USA comes second with 18 single corresponding authors and 10 multiple country publications. The most striking situation in Fig. 6(b) is that if the corresponding author is from Singapore, Poland, or India, then these papers do not have international collaborations and all authors are from the same country.

The contribution of authors and the number of articles published within a specific period or within a specific domain can easily be understood by Lotka's law illustration (Fig. S2).

According to Fig. S2, the gathered data are well-fitted and closely obeying Lotka's inverse square law (dashed line), which shows that the greater the number of publications, the fewer the articles published by a given author. Interestingly, we found that 309 authors from a total of 472 authors in the domain had only authored 1 FDI paper. This number is equal to 65.5 % of the total number of authors. The number of authors contributing with two articles was found to be 69 (i.e., 14.6 % of the total number of FDI authors) while that of authors contributing with 3 articles was only 43 (0.91 % of the total number of FDI authors). This result raises serious doubts about the continuity of research on FDI by experts in the field.

### 3.3. Journals publishing FDI articles

The most significant and popular sources for disseminating scientific findings are journals. Analysis of journals active in the publication of the results of a certain type of research field is a valuable method for authors to identify significant sources. In our study, we have included detailed analysis of journals publishing FDI results. Our analyses cover a wide range of evaluations, from the number of articles published by the journals to their impact. Fig. 7 shows the sources that provide the greatest coverage to the FDI process, and the number of papers published per year and global/local citations.

In Fig. 7(a) both numbers 10 and 11 share the same ranking, 10, with the same metric. It is clearly seen in Fig. 7(a) that *Desalination* journal showed more importance to FDI studies especially after 2018, in which a clear positive inflection was observed resulting in the 29 articles published during the year 2021. Desalination was also identified as the journal publishing most CDI articles [208]. Considering the strong link between CDI and FDI scientific community, and the scope of *Desalination* that includes emerging desalination technologies using thermal, membrane, sorption, and hybrid processes, it is coherent that the same

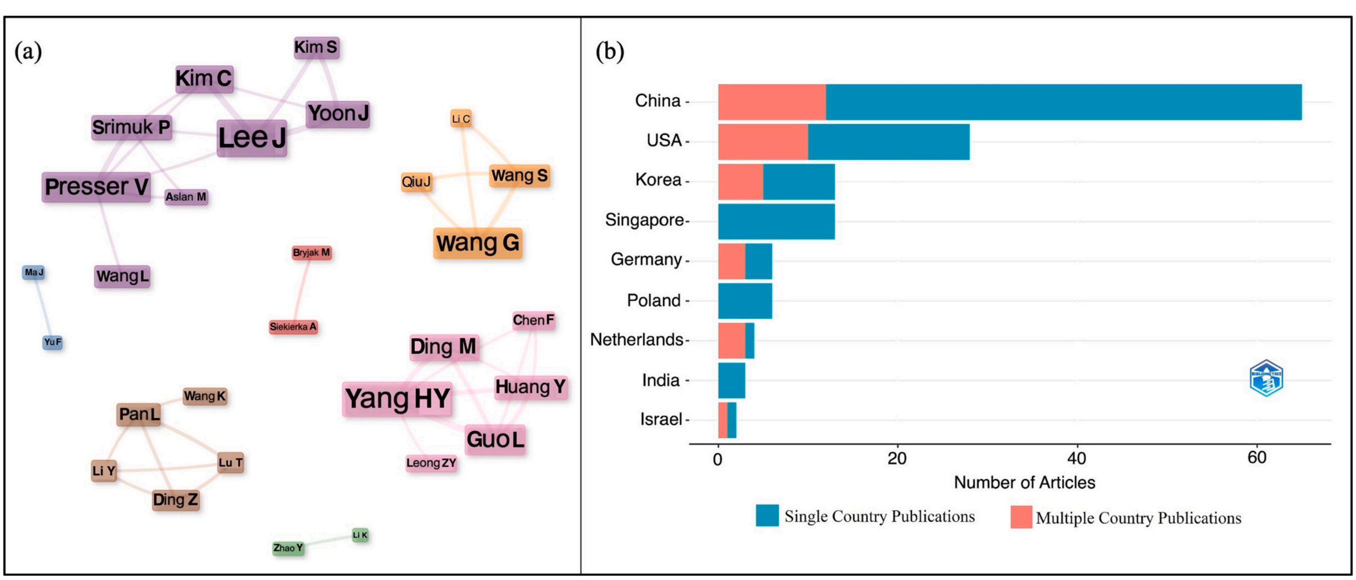


**Fig. 6.** (a) Collaborations between FDI authors (min. edges = 5) (b) top 10 corresponding author's countries.

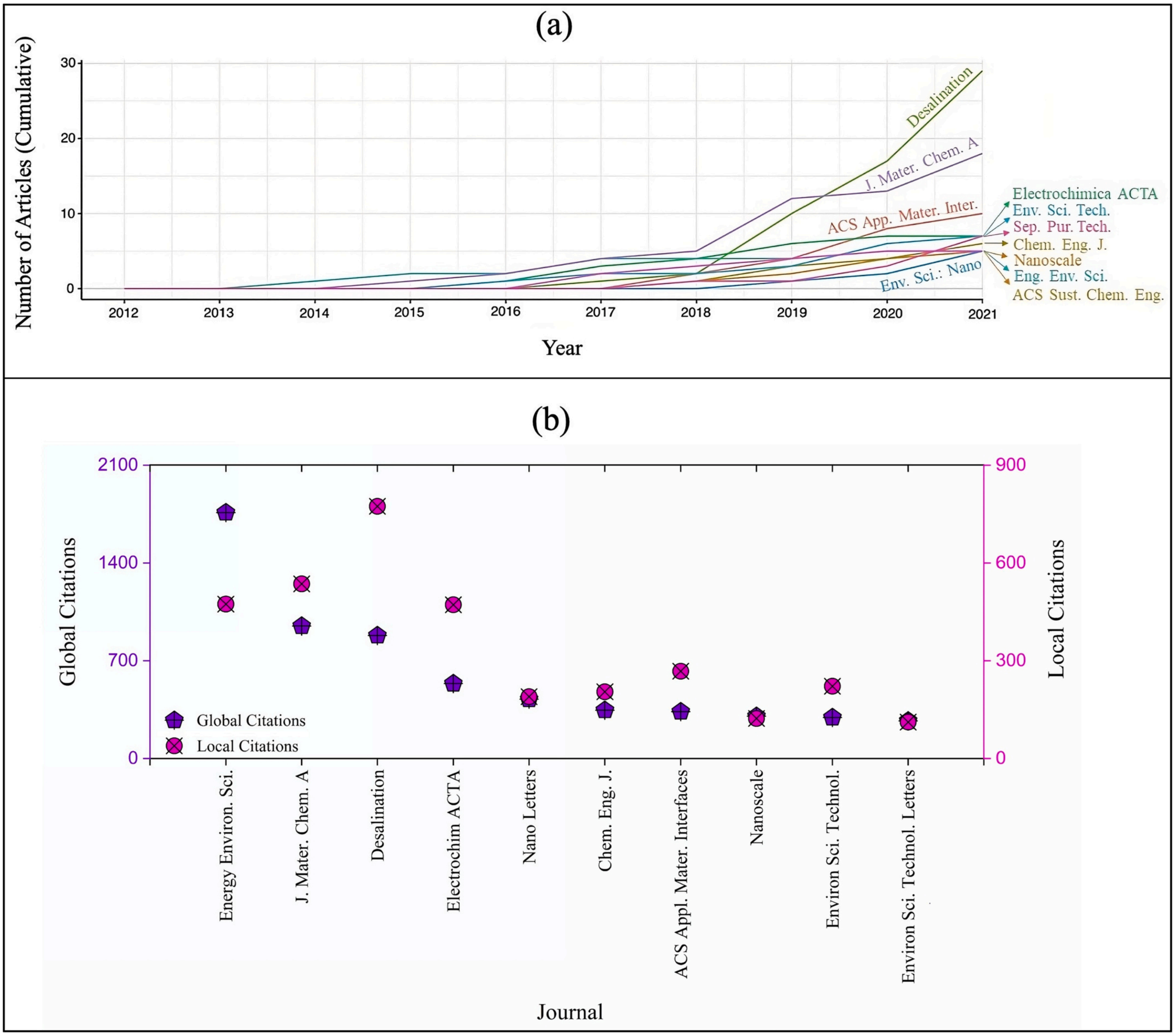


**Fig. 7.** (a) Top 10 journals more active in FDI publication over time (b) top 10 journals based on global and local citations.

journal is the leader in numbers of published studies in these fields. In addition, a thorough review of the FDI articles published in *Desalination* [116,225,228–230] indicates that special attention has been paid not only to new electrode materials but also to those studies focused on reducing the energy demand of the desalination process, either by reducing the operational voltage or by energy recovery [218,231,232]. In the second position of the most productive journals in FDI is *Journal of Materials Chemistry A* with 18 publications. This journal is focused on the synthesis and properties of innovative materials applied to energy and sustainability. Considering that many electrode materials tested for HCDI and FDI have been previously investigated for energy applications, *Journal of Materials Chemistry A* seems to be a good fit for those articles focused on advanced electrode materials such as molybdenum disulfide, hydrated vanadyl phosphate, trimetallic layer double hydroxides (NiVAl) or antimony/carbon composite [125,233–235]. In the third place ACS *Applied Materials and Interfaces* appears with 10 FDI articles mostly focused on elucidating the properties of new active materials for HCDI and FDI including $MnO_2$, PBA's, MXenes, or porous carbon decorated with bismuth nanoparticles [227,236–238].

Besides the cumulative number of articles published by each journal and the indices of performance, another significant parameter that measures the impact of published articles by a certain source is the number of citations. Fig. 7(b) presents both the global and local citations of top 10 journals. As can be seen in this figure, the most globally cited source is *Energy and Environmental Science* with 1761 citations. However, only 5 articles were published about FDI in the selected period, indicating the high number of citations per document (~352). Furthermore, this metric is also deeply affected by the vast number of citations obtained by just one of the articles published by Suss et al. [214] in 2015, that represents almost 60 % of the total citations received by the journal. *Energy and Environmental Science* is followed by *Journal of Materials Chemistry A* and *Desalination* with 949 and 881 citations, respectively.

Interestingly, the journal exhibiting the highest number of local citations in the collection is Desalination with a value of 774. *Journal of Materials Chemistry A* is ranked second with 536 citations and *Energy and Environmental Science* occupies the third position with 474 citations. The fact that journals are ordered differently in local and global citations could suggest that scientific content of the published articles is limited to these journals for local citations or broader for global citations.

A citation analysis is a reliable way to analyze the influence of journals where papers are published. The number of citations to a particular article in a given source indicates the importance of the article and ultimately its impact on the development of the topic. This situation directly shows the significance of the journal in which the article is being published by the scientific community. In our research, a separate investigation of the impacts of the journals based on *g*, *h* and *m* indices was conducted (Fig. S3). In accordance with the journal dynamics, Fig. S3 revealed that *Desalination* maintained the lead in the three metrics (*g*, *h* and *m* with values of 29, 16 and 2.667 respectively). The second source with the greatest impact in *h* (13) and *g* (18) indices were *Journal of Materials Chemistry A*, while the second place in *m*-index was taken by *ACS Applied Materials and Interfaces* with a value of 1.8.

### 3.4. FDI articles

Analysis of the published articles has the potential to show the hotspots and frontiers in the field to guide the readers. The citation numbers of an article demonstrate how a paper is used by researchers after its publication. The quantity of citations received by an article sheds light on the importance and the good reception within the scientific community. However, there are many factors that may affect the number of global and local citations. The older a published paper is, the more citations it accumulates. In addition, the open access status of the article and whether it is a review or research paper are also important factors influencing the cited values. In the present study, the articles with the greatest impact (top 10) in the FDI domain have been revealed by the number of their global and local citations (Fig. 8).

The most globally cited article, by far from the other articles in the collection, was entitled "*Water desalination via capacitive deionization: what is it and what can we expect from it*?". This review article, published in 2015 by Suss et al. (2015) in *Energy and Environmental Science*, received 1030 citations [214]. As it was discussed in the previous section, such a high number of citations results in a significant disruption in the list of most cited journals, especially when considering the important difference of articles published in each journal (29 in *Desalination* and only 5 in *Energy and Environmental Science*). This review, published by researchers from two main groups working in CDI and FDI processes, was one of the first-time battery materials that were mentioned in the literature as promising active materials to be used as electrodes for ion removal. Furthermore, drawbacks and concerns related with the long-term stability of the electrodes and the operation in complex mixtures of ions were also reported [214]. The second most globally cited article was entitled "*Hybrid capacitive deionization to enhance the desalination performance of capacitive techniques*" [112]. Published in 2014, this article received 393 citations, being 68 times cited in the FDI domain. However, the article published by Suss, et al. [214] in 2015, got 61 local citations. The published article in *Energy and Environmental Science* on HCDI by Lee et al. [112] in 2014, introduced the idea of combining a faradaic ($Na_4Mn_9O_{18}$) and a porous carbon electrode, as it was previously mentioned. Since these two last articles were published by *Energy and Environmental Science* journal, this result explains why this is the most globally cited journal in the FDI domain (Fig. 8). In the third position, we find the article entitled "*A Desalination Battery*", *published by Pasta* et al. *in Nano Letters in 2012*. This is considered the pioneering work that opened the path to combine non-carbon-based electrodes for water desalination [110].

### 3.5. Affiliations of FDI authors

It is useful for readers of articles to know the authors' affiliations and the provenance of the scientific knowledge in order to find out the hotspots of research studies of interest for any possible networks, collaboration, etc. If an institution has a high level of scientific research, it means that this field of research has strong scientific support and

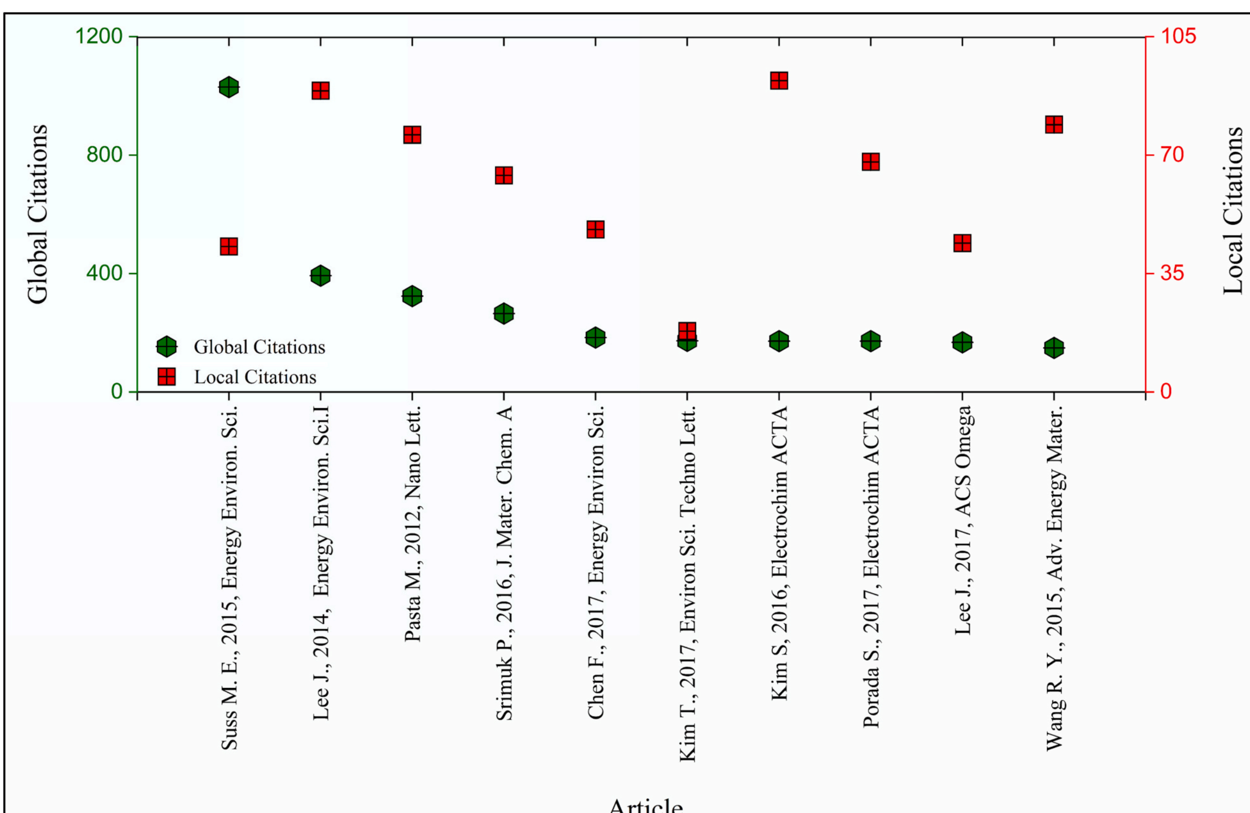


**Fig. 8.** Citations of top 10 articles in the FDI topic.

funding, and that future research in this area will advance significantly. Therefore, in addition to the most influential publications in the FDI field, it is noteworthy to investigate the institutions (i.e., institutes, research centers, universities, etc.) where research on FDI is most concentrated. Fig. S4 illustrates the top 10 affiliations with the highest interest on FDI and their yearly publications.

As previously stated, much interest in FDI has appeared since 2016. Singapore University of Technology and Design (SUTD) surpassed other institutions with a total of 66 FDI articles. The significant FDI productivity of this university is supported by the research developed by Yang H. Y., who is the author with the highest number of publications. Following SUTD, three Chinese universities appear in the ranking: Dalian University of Technology, East China Normal University and Ningxia University with 37, 36 and 35 published FDI articles, respectively.

Collaboration analysis is essential to reveal the networks and relationships of research groups and to guide researchers to find the most suitable institution to cooperate with. The obtained FDI teamwork is presented in Fig. 9.

The collaboration map from Fig. 9 reveals that there are 5 FDI established networks including only 2 or 3 affiliations. Dalian University of Technology and Dongguan University of Technology are the most predominant institutions in terms of publications due probably to the increased access to resources, research funds, academic and research infrastructures. However, Shanghai Ocean and Tongji Universities performed the most collaborations.

### 3.6. Countries with interest in FDI process

Top countries showing more interest in FDI technology can be found with the help of bibliometric analysis. When looking for postgraduate, pre-doctoral or post-doctoral positions abroad, it is important to know the expert research groups and the countries more active in a given topic. It would be beneficial to target countries that publish or cite more the topic of interest. In such a case, bibliometric analysis can reveal valuable information about the FDI field as it can be seen in Fig. 10.

Fig. 10(a) shows the frequency of articles published by the geographic distribution based on authors΄ affiliations. In this sense, the most effective country is China with a frequency of 416, then followed by USA and Germany with frequencies of 127 and 84, respectively. As mentioned above, three Chinese universities are among the top 5 institutions with the highest FDI output, which is clearly affecting this metric. On the other hand, the USA appears in the second position although only one of its universities, University of Illinois at Urbana-Champaign (with three principal researchers, Smith K. C., Su X. and Cusick RD), is among the top 10 most productive research centers. It should be mentioned that this result is also influenced by the work developed on FDI by some other relevant research groups such as those of Logan B. at Penn State, Whitacre J. at Carnegie Mellon and Santiago J. at Stanford University. When looking at the total citation metric (Fig. 10 (b)), China still ranks first with 1706 citations. The USA has received 1197 citations and Israel 1039 citations as of the date the dataset was downloaded. In the case of Israel, it must be highlighted the role of Suss M. in Technion – Israel Institute of Technology. As discussed above, being very active in both CDI and FDI research fields, Suss M. is the first author with the most cited article in the FDI literature analyzed in this study. Along with the publication of review articles about electrochemical technologies for water treatment [239], his research has focused on ion selectivity [76,240] together with the energy aspects of the technology [241,242]. More recently, a new electrochemical cell termed desalination fuel cell (DFC) was introduced by Suss M. claiming to continuously desalinate water while generating a significant amount of energy with only oxygen and hydrogen as fuel [243]. Fig. 10(c) illustrates the distribution of the average citations per article by country, which is a quantitative metric. In this assessment, Israel is far ahead of other countries with a value of 519.5. This country is followed by Australia and Japan with a value of 88 and 84, respectively.

Understanding the level of collaborations of the countries is very important in guiding early careers towards a certain field of research. In Fig. S5 we generated a collaborative cluster sketch to gain a better knowledge of the cooperative efforts of countries.

As can be clearly seen in Fig. S5, countries that conducted FDI research studies are divided into 2 main groups. The pink cluster with China in the center includes 9 countries (mainly in the Asia-Pacific region) in which the highest connection in this cluster is between Australia and China. Regarding this link, the group of Waite D. from the University of New South Wales (Australia) has played a significant role in this network by extending their knowledge in CDI and MCDI [244–249] to FDI studies [98,140,250]. Furthermore, an important point that should not be overlooked is that China has frequent collaborations with the countries in the blue cluster, which is formed by 14 countries and led by the USA, South Korea, and Germany. As it can be observed in Fig. S5, most connections are established between the triangle of these three countries, with the group of Presser V (INM—Leibniz Institute for New Material/Saarland University/Saarene—Saarland Center for Energy Materials and Sustainability) being the main connection point.

### 3.7. Text mining of FDI research

The bibliometric approach combined with text mining (TM) analysis


**Fig. 9.** FDI collaboration networks (min. edges = 2). (The bigger the node the more papers the affiliation has published and the thicker the edge the more collaborations between affiliations).

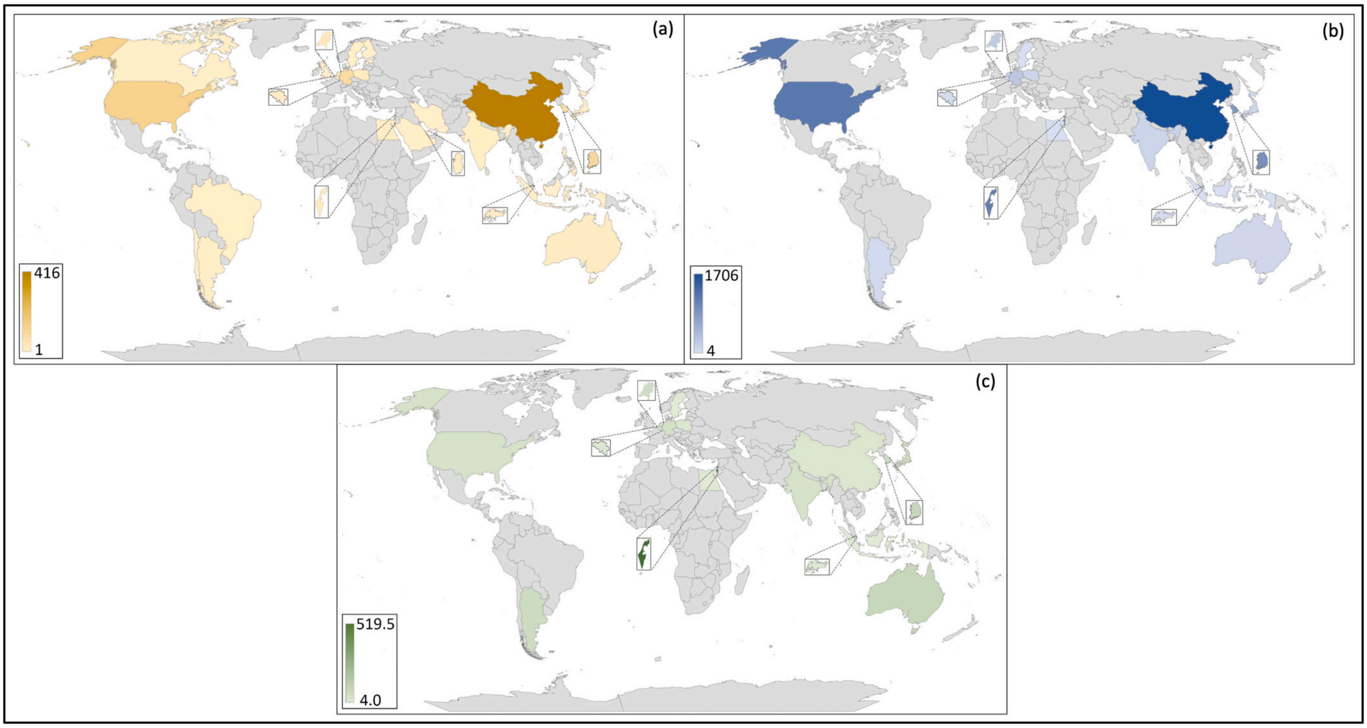


**Fig. 10.** Worldwide number of FDI published articles (a), total citations (b) and average citation per article (c).

helps to identify several essential research gaps for future development of FDI technology. Fig. S6 shows the word counts histogram of the FDI articles titles and abstracts with kernel density line to disclose the number of words the authors used to communicate their publications.

As can be seen in Fig. S6(a), authors usually used between 12 and 15 words in their FDI articles titles. The minimum, maximum, and average words of the titles are 3, 22 and 13.2, respectively. Fig. S6(b) depicts the word counts of the FDI articles abstracts. Authors mostly communicate their work using between 170 and 200 words in the abstracts of their FDI articles. It must be pointed out that a quite good number of journals limit the number of words of the abstracts. In this case, the minimum, maximum, and average number of words in the articles' abstracts are 53, 350 and 190, respectively. In this study, we would like to guide early careers, who pretend to work in FDI topics, demonstrating the importance of the title and abstract similarity analysis and how it can be conducted in the interested domain. In general, the title of a manuscript is usually the primary piece of information that readers pay attention to before deciding to continue reading or not. As a result, the authors must choose not only a title that captures the attention of researchers, but also a title that correctly explains the content of the work and attracts the audience to read further. The title of an article should be descriptive, not misleading, interesting, and most importantly unique. In addition, the abstract is an overview or a summary of the entire article. In some cases, the abstract of research articles are the only element of the study that is publicly available to readers. Therefore, this should be also clear, specific, unbiased, well-structured and have features such as the corresponding title [251]. Reviewers and editors may avoid articles with titles having similar wording to previously published ones, even if the content of the work is somewhat different. Similar titles may give a false judgment about the novelty of the study. In addition, coming up with an inimitable title will ensure that the work is displayed in more specialized clusters rather than large clusters when searching in databases like Scopus, Web of Science, etc. The use of text similarity methods is also important at the acceptance stage for editors. Text similarity approaches offer a way to compare the title and abstract of the article with those of other published articles in the field. The similarity results of titles and abstracts of FDI articles in a distance matrix form can be seen in Fig. S7. In this figure we presented only the pairwise word similarities, not the semantic similarities.

The similarity values obtained from the cosine distance number range between 0 and 1, where 0 means the two data instances are the same, while 1 indicates that the two data instances are different. When examining the title similarities (upper triangle), red tones are dominant in this area. In this case the average similarity distance value is 0.8775 indicating that FDI researchers have been very successful in naming unique titles to their studies so far. The cosine distance value of the two most similar titles was determined as 0.2174. When the abstract similarity values (lower triangle) are considered, it is seen that this area is predominantly yellow, and the calculated average cosine distance is 0.8027. Scholars working in the FDI field seem to be successful in summarizing their work with different sentence structures. This can be attributed partly to the FDI process novelty, and the high variety of battery materials proposed. In this case, the lowest cosine distance value is 0.2881.

Co-occurrence network graphs are invaluable tools for visually representing connections and interpreting meaningful conclusions about specific phenomena. The co-occurrence of author keywords provides key information about the field's conceptual structure. Fig. 11 specifies the co-occurrence map of the authors' keywords in the FDI domain.

As it can be seen in Fig. 11, the term “faradaic deionization” is still quite new and authors keep using mostly “capacitive deionization” or “hybrid capacitive deionization” which indicates the transition from the capacitive technology to first the combination of capacitive and faradaic and lately, pure faradaic electrochemical system. Fig. 11 also shows that terms such as “faradaic electrodes” “intercalation” or “desalination battery” have also certain relevance in the literature but with a significant minor frequency than the previous ones. Additionally, in each cluster appears keywords related to battery electrode materials (e.g., PBA's, MXene's or $NaTi_2(PO_4)_3$), showing the interest in employing different intercalation materials to optimize the FDI performance (i.e., salt removal capacity). Regarding the fields of FDI application, this analysis highlighted the importance of desalination as the main topic and included ion-selective applications represented by keywords such as “lithium selectivity”, “lithium recovery” and “ion selectivity”.

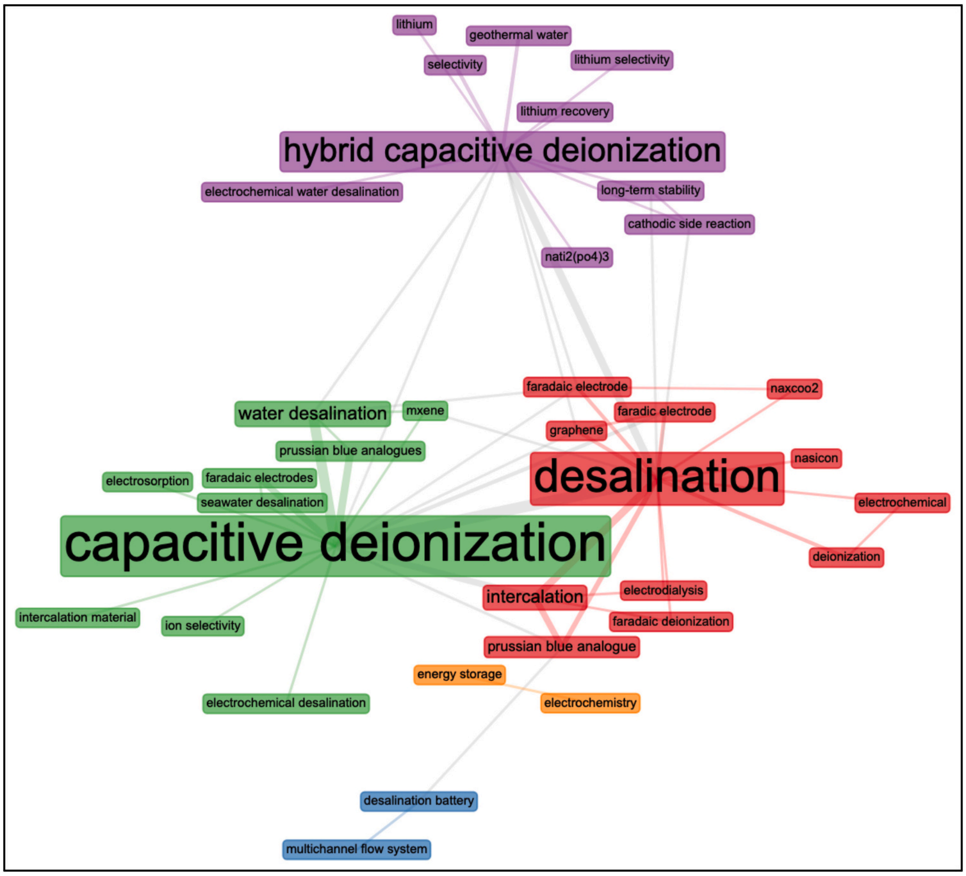


**Fig. 11.** Co-occurrence of author keywords (min. edges = 2). The centrality indicates the importance, the box size shows the citations, the strength of relations is specified by links, and each color represents a different cluster of co-occurrences.

Dominant words related to a specific content of a publication, like word cloud approach, are very helpful in identifying key themes in a field of interest. With the aim of complementing the analysis of the keywords, a word cloud approach was applied to find the most repetitive words in the abstracts and titles (Fig. 12). The more frequent the word, the bigger it appears on the graph. In the FDI field of research the top 3 dominant words in the titles were found to be "deionization", "capacitive" and "desalination" with counts 103, 85 and 67, respectively. In abstracts, words like "electrode", "desalination", "ion" are used 543, 401 and 363 times, respectively. This result points out again the influence of CDI technology as a starting point of the FDI studies, and the impact of the main FDI application, water desalination and ion removal. Also indicates that FDI researchers are specially interested in novel electrode materials.

To provide further evidence of important themes in the FDI field, we used a clustering approach to the abstracts. However, before clustering the abstracts, we performed an embedding process to convert unstructured textual data to structured numerical form. For this purpose, SBERT architecture in Orange was used. SBERT sentence embedding converted each document into a vector of 384 numerical values and then the structured data was clustered. By using the document embedding and clustering approaches, researchers can determine the semantic similarity of sentences (i.e., meaning similarity not word similarity). Document clustering enables us to extract local themes that are unique together with global topics that are common to all clusters. Clustering can help us identify latent groups in a document collection, thus we can then use the document grouping structure to find local themes specific to each group, as well as global topics shared by all groups [252]. In general, scientists can learn about areas of interest and prospective study directions through clustering approaches. In this study, the Birch clustering algorithm was used for clustering. Since the Birch method needs the number of clusters defined by the user, the silhouette score was used to find the most appropriate. The obtained results for different values are summarized Table 3.

Silhouette is a metric ranging from −1 to 1, where 1 indicates the best clustering and −1 the worst clustering state [202]. The highest silhouette score (0.1485) in Table 3 was obtained for 4 clusters. The resulting number of clusters are also an expression of the topics that FDI researchers are mainly interested in.

To find out the top 3 principal components to visualize the clusters in 3D scatter plot, ISOMAP dimensionality reduction method was employed. The distribution of the clusters in 3D space and the word cloud of clusters can be seen in Fig. 13.

Fig. 13 shows the data distribution in 3D space, and the scatter of clusters is sufficient to interpret topics in the collection. Cluster 1 shows the relevance of "desalination" as the main application of the FDI technology. Additionally, it links this application with the development of new "electrode" materials and the goal of reducing the "energy" consumption of the process. Cluster 2 refers to the aforementioned connection between FDI and CDI, being also relevant the use of "ion" either as part of the term "ion intercalation" or related with the concept of "ion removal". Cluster 3 highlights the importance of the "electrode" material and the high relevance of the material development in this topic. As it is common in many studies focusing on developing new active materials, "high" "desalination" or "ion" removal capacities are reported in the abstract. Cluster 4 reveals the importance of an emerging application in faradaic deionization, the capture of "lithium" from brines or waste streams using battery materials. Based on that idea, the term "recovery" has also a great importance.

Finally, sentiment and subjectivity analysis were conducted to figure

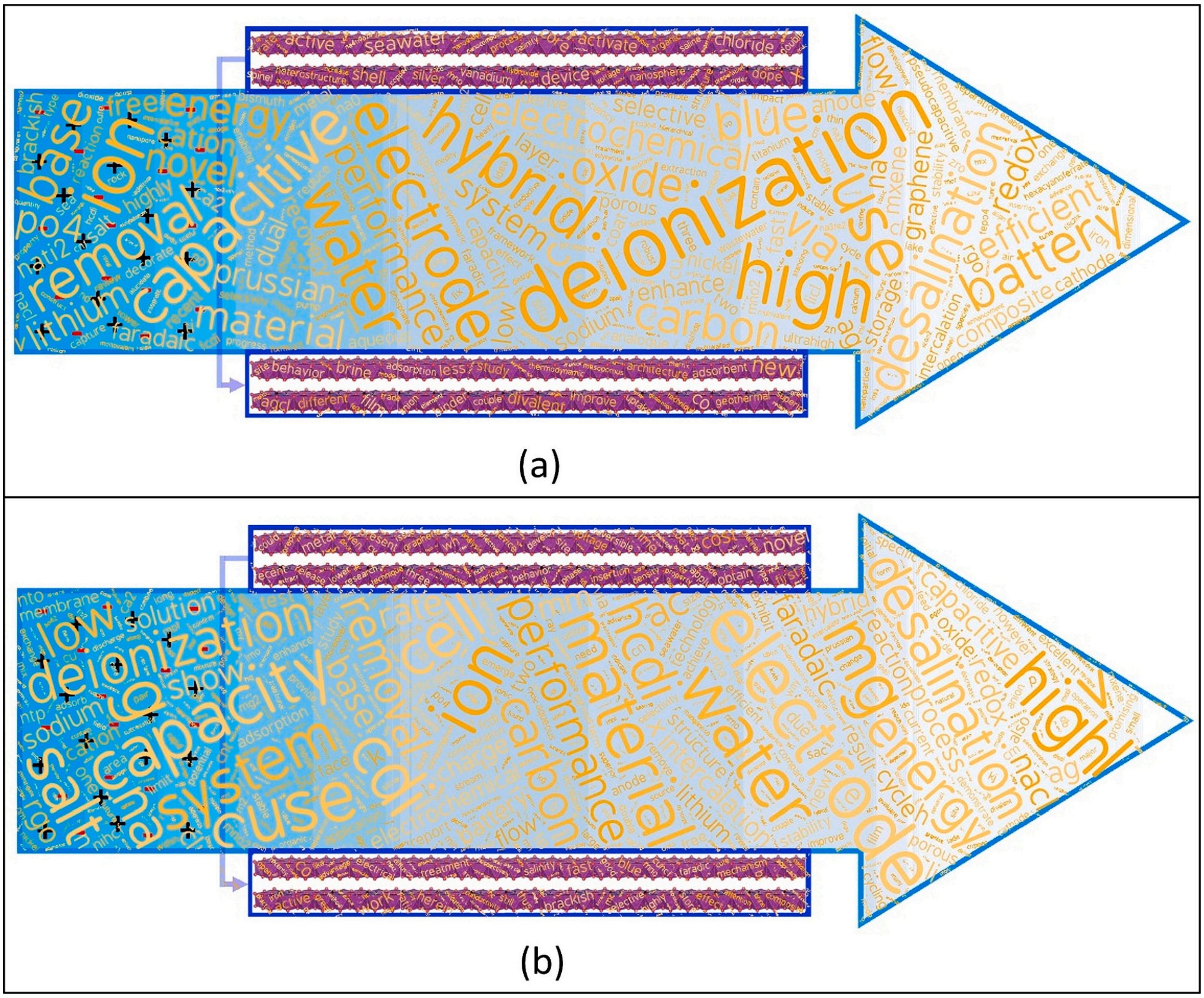


**Fig. 12.** FDI word cloud of titles (a) and abstracts (b).

**Table 3**
Silhouette scores of different cluster sizes.

| Cluster size (*K*) | Silhouette score |
|---|---|
| 2 | 0.1151 |
| 3 | 0.1372 |
| ***4*** | ***0.1485*** |
| 5 | 0.1331 |
| 6 | 0.1267 |
| 7 | 0.1291 |
| 8 | 0.1197 |
| 9 | 0.1234 |
| 10 | 0.0831 |

out whether the authors of articles were optimistic or not about their research studies and FDI technology in general; and to determine if they expressed their studies in a subjective or objective manner. The results were plotted in Fig. S8.

Fig. S8(a) illustrates the sentiments of the FDI authors from the provided abstracts of their articles. The majority, 128 articles, exhibit very high compound scores (0.81–0.89). While the compound score below 0.40 (optimistic) is about 92 %, nearly 5 % is neutral, and only about 3 % was pessimistic. These results prove that the new and groundbreaking FDI in the desalination field is a promising and auspicious technology. Besides, the minimum, maximum, and average compound scores of sentiment analysis were found to be −0.817, 0.993, and 0.805, respectively. Fig. S8(b) revealed whether the authors included their own opinions in the abstracts (subjective) or whether the texts contained facts (objective). Most of the FDI articles, 133 articles, were placed in the neutral zone (0.35–0.55). This indicates that researchers mainly consider a balancing factor when writing the abstract. Among these articles, 28 were expressed in a very subjective way, whereas only 9 articles were very objective. The minimum, maximum and average subjectivity scores were found to be 0.138, 0.763, and 0.479, respectively.

### 3.8. FDI technology outlook and recommendations for future research

It is worth quoting that the articles published during the year 2021 indicated that the major subtopic within the FDI literature is the research on electrodes chemistry and configurations including the use of additives, doping techniques and innovative preparation methodologies. A quick review of the articles published in 2022 and beginning of 2023 indicate that these topics remain as the most studied areas in FDI [253–261]. This outcome agrees with previous review analysis of CDI technology in which the research about different carbon materials, their modifications and the optimization of the electrode preparation have been deeply investigated [208]. After reviewing most recent publications in FDI one might realize that along with the interest on innovative inorganic materials such as MXenes [253,262–266], a new line focused on organic active materials (polymers) is attracting the interest of the FDI scientific community. This approach is oriented not only on studying

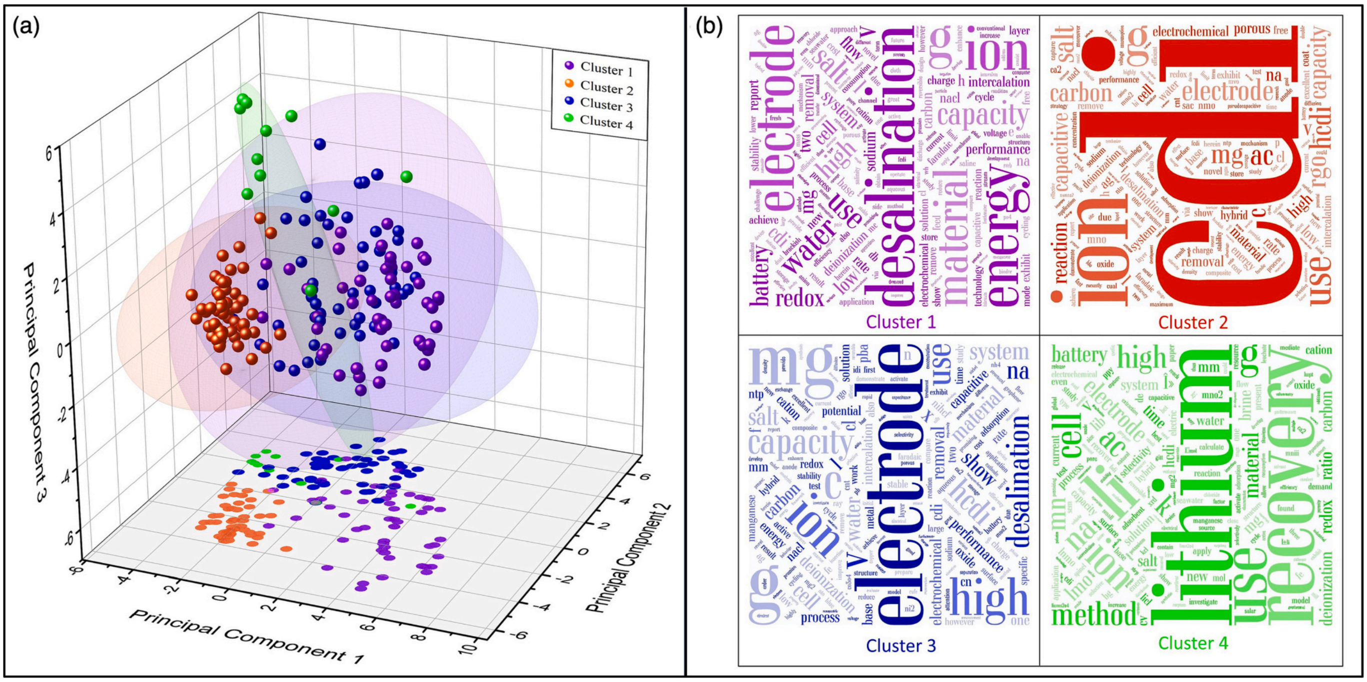


**Fig. 13.** Distribution of clusters (a) and word clouds of the clusters (b).

the use of new polymers [267–271], but also on doping those polymers to improve their adsorption capacity and long-term stability [38,128,272–274]. In general, it has been observed that a vast majority of articles published about electrode materials in FDI are focused on cation selective materials. Nevertheless, only a few anion selective materials (mainly silver and bismuth based materials, and more recently innovative CoFe LDH [275] as well as carbon-coated cobalt-iron alloy nanoparticles [276]) have been proposed. Besides, in this topic it is envisioned that research on anion-selective polymers such as porphyrins [277], macroporous polystyrene [278], modifications of polypyrrole (PPy) [279,280] or doped polyaniline (PANI) [281] might play a significant role.

An additional topic related to electrode development that has only caught the attention of a few is oriented to the durability of the materials. This is a critical aspect that has a tremendous impact on the feasibility of FDI technology due to its implications on the OPEX. Faradaic materials tend to have limited cycling stability due to the volume expansion and stress concentration of the material during the electrochemical process, which limits their further application for practical deionization. In this regard, it is highly desirable to develop strategies to address this problem. While quite a few studies have been focused on the long-term performance of carbon electrodes in CDI and MCDI [21,97–100,282–292], only a few stability analysis over cycling has been performed in FDI [262,293,294]. The team lead by A. Gorski and B. Logan from Pennsylvania State University has been the most active research group in this area, detecting the stability issues in some intercalation electrodes [282,295–298]. Recently, they observed that adsorption capacity reduction might occur when using PBA electrodes (CuHCF and NiHCF) due to the dissolution of electrode metals [296]. On the other hand, additional studies performed by the company Robert Bosch in collaboration with different research centers claimed that an excellent stability was obtained in NaCl solution for 500 cycles while the presence of Ca in the electrolyte solution led to a strong capacity decline due to the lack of stability of NiHCF, which forms crystalline precipitates [299]. Ding et al. [294], who incorporated additives in NiHCF electrode such as reduced graphene oxide, observed an improvement of the stability with a 78 % capacity retention after 100 cycles. Similar values were obtained by Gorski and Logan's research group when adding chelators in the synthesis of CuHCF [297]. Another strategy was followed by Bao et al. [300] based on the synthesis of an hierarchically structured NiHCF nanoframe (NiHCF-NF) electrode, which exhibited a large capacity retention of 88 % after 40 cycles intercalation/deintercalation. Other developed electrode materials include the stability of different crystallographic NMO electrodes [113] and a phase-integrated NMO [301], which showed high stabilities (over 90 % retention capacity) and salt adsorption capacities, 20–50 mg $g^{-1}$ and 65 mg $g^{-1}$, respectively. Furthermore, carbon-coated cobalt-iron alloy nanoparticles ($Co_3Fe_7$@C) achieved a great stability (100 % adsorption capacity retention over 100 cycles) [276] and MXene confined $MoS_2$ electrodes reached only 4 % desalination capacity degradation over 100 cycles [262]. Despite these studies, the integration of long-term performance experiments in the FDI studies has not yet been part of the regular tests conducted in FDI when novel materials are introduced. The authors of this paper consider that this kind of experiments should be encouraged with the aim of providing additional evidence about the stability of the electrode materials and the robustness of the performance.

Regarding the cell configuration, Redox Flow Desalination (RFD), an emerging technology inspired by redox flow batteries that uses redox electrolytes, has been gaining attraction since 2019–2020 because of its high desalination capacity (80–100 mg $g^{-1}$) [302–305]. Recent advances in this topic are related with the introduction of mediators [141,306], the scaling up of the RFD system [307], and the application to recover value-added organic compounds [308]. A novel approach to RFD is the solar-driven photoelectrochemical desalination in which photoelectrodes are combined with a redox flow electrolyte [138]. This technology bridges the gap between the advances in photoelectrochemistry and the latest developments in FDI. In addition, another significant trend is the use of hybrid reactors in which the combination of electro-separation and electro-conversion processes is proposed for simultaneous wastewater treatment and critical materials recovery [239,309]. A great example of the synergies achieved by the hybridization of these technologies was shown by Kim et al., who used an asymmetric system integrated by an intercalation material (LMO) and a well-known electro-oxidation electrode (Boron-doped diamond, BDD) for simultaneous removal of organic pollutants and lithium capture to treat the industrial wastewater of a battery recycling plant [310]. More recently, Sun et al. [311] employed 3D titanium nitride nanorods composite to achieve an excellent removal of heavy metals by coupling faradaic-reaction and electro-adsorption. Here, a new generation of novel design hybrid electrochemical cell reactors is envisioned using advanced electro-conversion electrodes with a high stability combined with innovative ion/molecule capture materials that could be applied to relevant fields. Aligned with this idea is the HYSOLCHEM European project also focused on the development of a hybrid cell equipped with a photocathode and a "dark" anode with the aim of treating wastewater while fixing $CO_2$ and producing added-value chemicals. In this case, ion separation or capture is not proposed although researchers involved envisioned potential modifications that could enable this feature.

Regarding FDI applications, the huge demand for energy storage devices, and more precisely lithium-ion batteries, are also driving some other topics, such as the introduction of electrochemical technologies for lithium capture [147,312–315]. This strategy has been proposed in two different scenarios: i)- the capture of lithium from brines [316–319] and ii)- the recycling of the batteries [313]. In the first case, battery-like materials such as $LiFePO_4$ (LFP) and $LiMn_2O_4$ (LMO), have been successfully tested at the laboratory scale although still lacking for larger systems working at higher TRL's [147,313]. Regarding battery recycling, the objective is to recover the most valuable components such as cobalt, nickel and lithium. In this sense, the use of FDI technology equipped with active electrode materials specially designed for lithium capture has been proposed as one of the most promising technologies [147,313]. Along with these applications, nutrients recovery [308,320] and organic pollutants capture, and conversion are emerging as new topics of research linked to the development of FDI technology.

Finally, a proof of economic feasibility is also critical for commercialization of electrochemical systems. Despite the initial lack of this kind of studies in the CDI and FDI fields, during last five years, there has been an increase in the number of publications on life cycle assessment and technoeconomic analysis [321–331]. Still, most of those publications are related with CDI and MCDI, being the work published by Metzger et al. [321] and the successive comments and replies, the most comprehensive study in the FDI field [321,326,327]. As a critical finding, Metzger et al. [321] shows in their techno-economic analysis that the costs of electrodes (preparation of active material and electrode processing) and, specially, the presence of ion exchange membranes are key contributors to the overall capital and operating costs. However, most of these analyses have not considered other critical aspects such as the electrical configuration of the cell. This will affect the costs of the power electronics of a multicell-stack, and the energy consumption of the electrochemical system as a consequence. Therefore, a comprehensive technoeconomic analysis incorporating this evaluation is needed for assessing feasible electrochemical approaches for water treatment.

## 4. Conclusions

In this age of information explosion, it is becoming increasingly difficult to become a lead author/affiliate/country on a topic and present the latest study findings to the scientific community as quickly as possible. To achieve these successes, the effective use of bibliometric and machine learning (ML) methods is gaining importance by the day.

In the present study, we examined the faradaic deionization (FDI) domain, which is still in its infancy, with bibliometric, ML, and text mining (TM); and tried to guide researchers working in FDI or early careers in this field. FDI is an emerging technology that finds inspiration in the energy storage field, mainly on the active materials employed for battery applications. The extension of the ion adsorption capacity together with the higher selectivity of battery materials in comparison with capacitive carbon materials, typically used in CDI, have boosted the interest of the scientific community in this technology. This is so, especially since 2016, when relevant studies on new battery electrode materials were applied to water deionization.

The number of published FDI articles in journals as of September 30th, 2022, is only 170, with the first FDI article reported in 2012, indicating that FDI is a newly developed technology. The annual growth rate of this research field is at a very high level (55.12 %) and the average citations per article is also quite high, 46.69. These values demonstrated that FDI is gaining more attention in the scientific community. In terms of number of fractionalized publications, *g* and *h* indices, Lee J. and Yang H. Y. are the leading scientists of FDI. The collaboration network of authors indicates that there are 7 working groups focused mainly on FDI. This was calculated based on at least 5 collaborations. China and the USA are the leading countries for FDI research. The average citation per article points out that Israel is in first place. The 3 journals that mostly include scientific studies on FDI are *Desalination*, *Journal of Materials Chemistry A*, and *ACS Applied Materials and Interfaces*. The most cited article on a global basis, with 1030 citations, was published Suss, et al., (2015) [214] while the most cited article locally, with 68 citations, was published by Lee, et al. [112] in 2014, Singapore University of Technology and Design (SUTD) stands out as the institution with the most articles published on FDI. Data mining results show that titles of FDI publications mostly include 12 to 15 words while abstracts contain 170 to 200 words. Co-occurrence of author keywords revealed that FDI articles were communicated with words capacitive deionization, desalination and hybrid capacitive deionization providing links about electrode materials used and application areas. With the word cloud approach, the most preferred words by the FDI researchers. In titles "deionization", "capacitive", "electrode" and in abstracts "electrode", "desalination", "ion" were the top 3 words. It is important to note that the term "faradaic" is not the most employed since most of papers still refer to it as capacitive deionization even though battery-type materials are considered. Similarity analysis of the articles' titles indicated an average similarity of 0.8775, demonstrating therefore that the titles are quite different and that the FDI authors were able to find unique titles to communicate their studies. The different themes in the FDI field were revealed by applying the Birch clustering algorithm to the abstracts of the articles. Clustering results show that researchers are mainly interested in lithium recovery, electrode material production, desalination application and comparison of FDI with CDI. A sentiment analysis was conducted to quantify the authorś belief in FDI technology, and the results indicate that researchers are highly (~92 %) optimistic about FDI and have a positive outlook on the future of this technology. Subjectivity analysis specifies that the authors in the abstracts of their articles are neither objective nor subjective but are in a neutral zone (133 articles have a score between 0.35 and 0.55).

The FDI has a long way to go with room for improvement. As this area evolves, its bibliometric, data mining and ML imprint may be followed through previous obstacles to future advances. Overall, this investigation provides several valuable insights to early careers, researchers, and educators in the FDI domain.

## CRediT authorship contribution statement

During the preparation of this work the authors used OpenAI's text-to-image-generation architecture, DALL-E 2 to create the graphical abstract. Upon generating the draft image, the authors edited the image, and they took the ultimate responsibility for the content of the publication.

## Declaration of competing interest

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

## Data availability

Data will be made available on request.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.desal.2023.116715.

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