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REVIEW

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Combinatorial high throughput methodologies: the potentials in heterogeneous catalysts synthesis, screening and discovery—a review

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Abstract

Background Catalysis represents a critical field that greatly contributes to human living, technology, economic growth and the environment. Compact catalysts have frequently been applied in manufacturing a range of substances and fuels, thus essentially subsidising income and good living. Catalysts offer significant ecological profits, such as catalytic transformers, fuel cell technology, chemical production and environmental cleaning in automobiles. Still, the use of catalysts is anticipated to raise due to the need to discover ecologically responsive production pathways and affordable products.

Main body of the abstract Since its discovery, catalysis has played a vital role in a range of fields, from industrial production, sustainable energy strategy and environmental cleaning to the pharmaceutical industry. The discovery and use of catalysts mark a critical aspect in chemistry due to the raising need for greater output plus effectiveness in industry and cleaner production. Despite their importance, the invention of catalysts remained a challenge as it relied on trial-and-error tactics. Customarily, catalysts were developed using various tiresome, time-wasting and usually one-at-a-time techniques characterised and screened for activity and modified until no extra improvements were necessary. However, with the advancement in science and technology, catalyst discovery has been made more accessible and faster through combinatorial techniques. Combinatorial experimentation technologies in chemistry are a fast emerging field that includes the formulation and fast creation of a combination of material libraries and parallel screening for particular chemical or physical characteristics of concern in a general economical and compelling style. These techniques in heterogeneous catalysis are essential for the quick invention of catalysts and for improving the available ones. The rapid and economic invention of catalysts and optimisation of the available ones attract much industrial interest.

Short conclusion The present review uncovers catalysis development, progress, history and some applications. The latest developments and challenges associated with using high throughput experimentation techniques in synthesising, optimising, discovering and screening catalysts are discussed. A high throughput experimentation approach is potential in catalysis and is promising.

Keywords Catalyst, Catalysis, Combinatorial methods, High throughput technique

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Background

Main text

Benefits of catalysis

Catalysis is a known aspect of human history that has attracted diverse use in different industries, energy creation and ecological conservation (Escayola et al. 2024; Scheidtmann et al. 2001). Studies show that 90% of chemical output pathways rely on at least one catalytic stage (Armor 2011; Baerns and Holena 2009; Farrusseng 2008; Kerby et al. 2005; Volpe and Lugmair 2020). Using catalysis in industry lowers manufacturing expenses and by-products, thus assisting in retaining resources (Scheidtmann et al. 2001). Economically, reports show that catalysts are applied in the manufacturing of about 7000 molecules, costing more than USD 3 trillion globally, where the production involving catalysts constitutes about 60% of chemical manufacturing and 90% of pathways (Liu et al. 2022a, b; Senkan 2001).

Besides, the numbers are forecasted to increase because of the raising need for the invention of ecologically responsive production pathways (Liu et al. 2022a, b). Reports indicate that the annual contribution of goods and services linked to catalytic processes to the global economy exceeds USD 10 trillion (Volpe and Lugmair 2020). In 2013, the global market for catalysts was predicted to be worth USD 20 billion, and by 2024, that market is anticipated to have grown to nearly USD 34 billion (Volpe and Lugmair 2020). Based on the importance of catalysis, optimisation of existing catalysts, new discovery, rapid and parallel synthesis, and screening of catalysts are paramount and require fast-tracking (Allen et al. 2019; Farrusseng 2008; Isbrandt et al. 2019; Kerby et al. 2005; Welch 2019; Zhang et al. 2020).

Catalysis development

The field of catalysis has grown quite remarkably over the years. The growth ranges from the discovery via different tiresome, time-consuming and often one-at-a-time techniques characterised and screened for activity and total modification to modernised and fast discovery methods (Hampson et al. 2024). Therefore, the development of new catalytic materials has benefited more from the development of high throughput techniques (Allen et al. 2019; Compton et al. 2019; Ehm et al. 2020; Hattrick-Simpers et al. 2015; Isbrandt et al. 2019; Liu et al. 2022a, b; 2019; Maier 2019; McCullough et al. 2020; Wills et al. 2021; Yao et al. 2020; Zang et al. 2022). Combinatorial chemistry is a quickly evolving area that encompasses the formulation and quick creation of a combination of material libraries in conjunction with parallel screening for particular chemical or physical characteristics in an economical and practical approach (Hampson et al. 2024; Ehm et al. 2020; Isbrandt et al. 2019; Jandeleit et al. 1999; Lindstrom and Pettersson 2003; Maier 2019; Senkan 2001; Turner et al. 2009; Williams et al. 2019; Wills et al. 2021). The rapid and low-cost invention of catalysts and improvement of available ones is vital in industrial manufacturing, environmental cleaning, sustainable energy generation strategy and the pharmaceutical industry. The blending of rapid and efficient industrial approaches is key to the economical creation of catalytic material libraries that are crucial in various utilisations (Maier 2019; Tsapatsaris 2008; Williams et al. 2019). Studies show that a sum of catalysts in industrial applications, both heterogeneous and homogeneous, was invented via some form of combinatorial approach (Maier 2019; Newsam and Schuth 1999). The current review unveils the progress, history, current status and challenges associated with the utilisation of high throughput combinatorial techniques for rapid invention and screening of heterogeneous catalysts.

Progress of high throughput combinatorial technology application

Chemistry has historically relied on single experiments, which continues to be predominant in most academic laboratories today (Maier 2019; McCullough et al. 2020; Williams et al. 2019). Findings from such experiments are then used to guide the design of subsequent experiments. They are highly speculative and lead to a plodding pace of development for the industry at issue when novel active materials are developed empirically using trial-and-error approaches on a small number of selected samples (Baerns and Holena 2009; Farrusseng 2008; McCullough et al. 2020; Volpe and Lugmair 2020; Yao et al. 2020). This study approach which is based on thorough research and comprehension takes much time. Thus, to make progress and re-energise the chemical research community, new research methodologies must be created (Farrusseng 2008; Yao et al. 2020). A practical substitute is the combinatorial high throughput technique. The technology has a long historical foundation in speeding up research and innovation (Farrusseng 2008; Maier 2019). Edison, 1878, Mitasch 1909 and Ciamician, 1912 made early applications of high throughput testing according to sources (McCullough et al. 2020). Parallel experimentation on libraries frequently saves time and money.

Accelerating research and development with combinatorial methods is well-established and included in many businesses' product portfolios today (Welch 2019). The first ammonia synthesis catalyst was discovered by Mittasch et al. at BASF in 1909, followed by a "systematic investigation of the periodic table" involving roughly 20,000 experiments. Combinatorial high throughput approaches are rooted in discoveries made throughout the twentieth century, and one of the most notable

examples is the first ammonia synthesis catalyst (Farrusseng 2008). High throughput screening technologies were applied in catalysis and led to the discovery of the first Haber–Bosch catalyst in 1913 after meticulously examining over 2500 possible catalysts and conducting 6500 trials. Iron was eventually chosen as the catalyst as a result of this process (Hattrick-Simpers et al. 2015). Ziegler found this method appealing and used it to find the polymerisation catalysts in the 1950s (Farrusseng 2008).

Hanak's groundbreaking work in the 1970s resulted in high throughput technology. At the RCA corporation laboratories, he created and implemented what are now known as composition-spread or gradient libraries for research and innovation (Hanak 1970; McCullough et al. 2020). His efforts successfully helped several innovative items enter the market (Farrusseng 2008). High throughput technology was first developed in the 1970s under the name "Multiple Sample Concept" (Hanak 1970; Hendershot et al. 2005; Liu et al. 2019). Hanak observed that "the single experiment technique is expensive and ineffective because it improperly utilises the highly skilled researcher's time and effort" at the time (Farrusseng 2008). Hanak created the first gradient library using physical vapour deposition techniques to pursue novel super-conducting alloys, photovoltaic materials and other materials.

However, due to the lack of trustworthy technology for more widespread uses and the infant stage of informatics and robotics, his concept was long neglected by industry and academics. The late 1980s emergence of powerful personal computers capable of automating data collection and processing, as well as the remarkable success of pharmaceutical companies in novel medication development via parallelised synthesis and screening, caused a resurgence of interest in the 1990s (Farrusseng 2008; Hattrick-Simpers et al. 2015; Pereira and Williams 2007). However, laboratories for materials and life sciences used high throughput technologies (Allen et al. 2019; Farrusseng 2008; Nicolaou et al. 2002).

Combinatorial chemistry and high throughput screening methods for research were adopted by the pharmaceutical industry in the 1980s to accelerate the drug discovery process, which at the time was slowed down by high costs and protracted development times (Nicolaou et al. 2002; Volpe and Lugmair 2020). Successful medications developed employing high throughput combinatorial technology have been reported in life science (Mennen et al. 2019; Vittoria et al. 2022; Volpe and Lugmair 2020). It is now widely accepted that such combinatorial research involves more than just doing numerous tests simultaneously. The application of combinatorial methods in the life sciences began in the middle of the 1980s, 14 years after Hanak. Geyson released the first spatially resolved 96 peptide library in 1984 using parallel peptide synthesis on microtiter plates, and Houghten described the tea bag approach in 1985 (Maier 2019). The library of putative superconductors and its screening by the biological chemist Schultz was published in 1995, and this paper served as the impetus for high throughput and combinatorial materials research.

Moates used infrared thermography to depict the heat of H_2 combustion on various catalysts in 1996 (Maier 2019). In 1997, Symyx Technologies published a library of more than 25,000 different compounds, capturing the state of the art in combinatorial chemistry (Farrusseng 2008). High throughput technology expanded quickly in numerous laboratories worldwide after 1998, and diverse high throughput characterisation techniques, including spatially resolved mass spectrometry, gas chromatography, conductivity and more, have been reported since then (Maier 2019). High throughput library synthesis, automated performance measurements, data gathering and evaluation, and thorough library design based on literature and data collection information are all required for a successful strategy.

Indeed, many early-stage research teams in academia or industry who developed their method were able to satisfy these requirements (Farrusseng 2008). The cost of installing and maintaining such a comprehensive workflow is so high that only industries can afford it, making it almost unaffordable for University laboratories (Maier 2019). Not just in the late 1990s, but even now, there is some scepticism against combinatorial techniques in materials research, which is not without justification. But the idea caught hold, and high throughput technology entered numerous laboratories. The early focus on the development of novel technologies, as well as the identification of novel materials and catalysts, led to a flood of patents and publications. However, these early experiments have reported no new commercial catalyst-based method.

There has been a hunt for new catalysts for several dream reactions, including the air oxidation of propene to propylene oxide, the direct amination of benzene with ammonia and air, the air oxidation of benzene to phenol and many others. This early lack of accomplishment was viewed as a failure of Combichem's first material promises (Maier 2019). The development of high throughput technology took place as the emphasis shifted from new discoveries to the advancement of already-known catalysts and materials. A study of the quickly evolving field of high throughput technology for synthesising materials was made available in 2005 (Maier 2019; Takeuchi et al. 2005). Subsequently, there has been a notable increase in the use of high throughput experimentation for developing and studying heterogeneous catalysts in particular (Hendershot et al. 2005).

High throughput technology has been developed for and applied to a variety of materials since the year 2000, such as electronic and magnetic materials, polymer-based materials, optical materials, biomaterials, paints, drug formulations, detergents, cosmetics, glues, corrosion-resistant materials, electrocatalysts and heterogeneous catalysts, leading to a dramatic increase in the number of related publications and patents (Aljohani et al. 2012; Emmanuel et al. 2019; Farrusseng 2008; Guerin and Hayden 2006; Guerin et al. 2004; Guerin et al. 2006a, b, c; Guerin et al. 2006a, b, c; Nicolaou et al. 2002). Since its discovery, catalysis has revolutionised several fields including the chemical industry, environmental safety, oil and gas and pharmaceutical industry.

Catalysis in the chemical industry

Over the years, catalysis has enjoyed diverse applications and offers much utility in the chemical industry. It is a critical component in converting toxic molecules like carbon monoxide into harmless or environmentally unfriendly molecules such as carbon dioxide into valuable products. The use of CO from the reverse water gas shift reaction in several chemical reactions has been made possible by catalysis (Nielsen et al. 2018). Studies indicate that the global overdependence on fossil fuels-based energy sources has caused the excessive emission of carbon dioxide gas, which is associated with climate change, particularly global worming (Arroyo and Miguel 2019; Chai et al. 2022; Ribeiro and Junior 2023).

The reverse water–gas shift reaction is a chemical process that converts carbon dioxide to CO via deoxygenation of CO_2 to CO, which is catalysed by transition metals producing water when dihydrogen is present (Nielsen et al. 2018). The transformation of carbon dioxide into value-added molecules by using different catalysts has been well addressed (Kattel et al. 2017). Reports show that methane production is selectively facilitated by catalysts like Ni/ZrO_2, $Rh/\gamma Al_2O_3$ and $Co_4N/\gamma Al_2O_3$, which exhibit excellent efficiency in reducing CO_2 up to 98–100% conversion (Beuls et al. 2012; da Silva et al. 2012; Razzaq et al. 2015). In addition, ruthenium catalyst at high CO_2 and H_2 pressure in N-methyl pyrrolidinone has been used to generate CO to convert olefins to alcohols using the reverse water gas shift reaction (Nielsen et al. 2018).

A preliminary hydroformylation and a subsequent reduction are required for transformation to reach the appropriate alcohol. Styrene and stilbene showed poorer efficiency with the predominance of reduced alkene production, while cyclooctene and other hexene regioisomers could be converted to the required alcohols with a yield of up 70–80% (Franke et al. 2012). Still, an official Rh-catalysed reverse water gas shift reaction has been reported, transforming olefins into the corresponding aldehydes (Nielsen et al. 2018). The transformation involves the formation of a bidentate phosphine ligand that is substituted with pyrrole, which, combined with excess CO_2, prevents the aldehyde from decomposing. Additionally, this ligand inhibited undesirable side reactions, including the hydrogenation and isomerisation of the alkene. It offered strong regioselectivity, and the reaction could be carried out under lower pressure at 100 °C than the methods used to obtain alcohols and amines (Ren et al. 2017). Besides, researchers could create carboxylic acids and the required products by adding carbon monoxide and water to olefins at 180 °C with an Rh catalyst. The promotion of this reaction required the presence of an iodide source and an acidic promoter. Studies show that several cyclic and noncyclic olefins can be hydrocarboxylated to give the corresponding acids in a yield as high as 62–91% at high pressure (Ostapowicz et al. 2013). There is a report on the use of alcohols in the hydrogen-producing reverse water gas shift reaction at high temperature (160 °C) and CO_2 pressure in the ionic liquid 1-butyl-3-methylimidazolium chloride (Nielsen et al. 2018). $Ru_3(CO)_{12}$ was used as the catalyst to thoroughly study the methodology's scope and limitations by using a variety of olefins and alcohols. Notably, ethylene can change into methyl propionate, a crucial step in the Lucite Alpha process that synthesises methyl methacrylate for industrial use (Nielsen et al. 2018). Methyl propionate is a fundamental component in polymer chemistry. The idea was then modified to use supercritical carbon dioxide in a continuous flow configuration (Stouten et al. 2016; Wu et al. 2014).

There are also reports on the reduction of CO_2 to CO via homogeneous and heterogeneous electrochemical reduction using molecular catalysts comprised of metal centres (Francke et al. 2018; Zhang et al. 2017). Besides, Fe- and Cu-based catalysts have been used in converting CO_2 to methanol, a valuable precursor for many important compounds (Tursunov et al. 2017). Besides, nanostructured precious metals, including Au, Ag and Pd, have been investigated for CO_2-to-CO conversion in water. These metals are engineered with varying shapes, sizes and compositions ranging from nanometers to micrometres (Zhang et al. 2017). Reports show that dimethyl ether can be synthesised from CO-rich synthesis gas using a supported bimetallic nanoparticle catalyst (PdZn), which showed excellent activity and selectivity (Gentzen et al. 2019). Generally, catalysis is a driver of the current chemical industry and will continue to play a vital role in the field.

Catalysis in environmental protection

Global population growth triggers many concerns about environmental pollution due to increased anthropogenic activities. With environmental regulations in place since the 1970s, there has been a noticeable decrease in the emissions of carbon monoxide, unburned non-methane hydrocarbons, oxides of nitrogen and total particulate matter as a result of ongoing advancements in the treatment of automobile exhaust emissions (Farrauto et al. 2019). This has been made possible through catalytic converters to prevent these pollutants from getting into the environment (Farrauto et al. 2019). On the other hand, plastic pollution is among the pollutions that threaten environmental safety (Ratnasari et al. 2017; Rehan et al. 2017; Pawelczyk et al. 2024).

Therefore, emerging strategies for recycling and upcycling are being developed in response to the environmental crisis brought on by plastic pollution (Ellis et al. 2021; Ratnasari et al. 2017; Rehan et al. 2017). Plastics made from fossil fuels are now widely used by humanity, and reports show that 8.3 billion metric tonnes of plastics are thought to have been produced up until 2015 (Jambeck et al. 2015). It is anticipated that synthetic polymers will linger in landfills for millennia to centuries due to their extraordinary resilience. Furthermore, the release of plastics into the environment is a major cause of pollution worldwide, and it is estimated that between 4.8 and 12.7 million metric tons of plastics end up in the world's oceans annually. Plastics are now mostly recycled mechanically into usable materials via two basic processes: primary (post-production) and secondary (post-consumer) to overcome this problem.

While recycling rates differ from nation to nation, the global average is low, 16% in 2018 with 66% of plastics thought to be disposed of in landfills or released into the environment (Nicholson et al. 2021). Chemical recycling offers opportunities to address this challenge by depolymerising plastics into intermediates that can be used to synthesise the same plastic with virgin-like material properties. They can be converted into another material or upcycled if the final product is more valuable (Garcia and Robertson 2017; Pawelczyk et al. 2024). This method of converting plastic trash into circular material streams through catalysis differs significantly from converting plastics into fuels or energy recovery. The potential creation of value-added goods outside the purview of mechanical recycling is made possible by chemical recycling. These tactics are essential to creating a new paradigm where a plastic's first usage is just one stage of its useful life (Garcia and Robertson 2017). Still, reports show that the pyrolysis of waste plastics using zeolite-based catalyst in conjunction with pyrolysis improves the plastics pyrolysis process and provides a higher-grade liquid fuel that may be utilised as premium fuel in fleet engines (Ratnasari et al. 2017; Liu et al. 2020a, b); Luo and Feng 2017; Rehan et al. 2017). However, pyrolysis of Municipal solid waste using catalysts has been reported to produce high-grade pyrolysis fuel (Liu et al. 2020a, b; Sipra et al. 2018).

Besides catalysis plays a more significant role in the catalytic conversion of carbon monoxide over supported metal nanoparticles such as Cu, Ni, Au and platinum group metals as it is practically applied in interior air cleaning and car exhaust emission management (Emmanuel et al. 2019). Studies indicate that supported noble metal nanoparticles are an appropriate catalyst for the catalytic conversion of volatile organic molecules, which is a tactic for eliminating environmental pollutants (Guo et al. 2021). Silver, gold, palladium and platinum-based nanoparticle catalysts are reported as suitable for $NaBH_4$-assisted nitrophenol reduction, a highly poisonous and carcinogenic chemical thought to be a common refractory water pollutant and environmentally hazardous material (Liao et al. 2019). Besides, catalysts for catalytic reduction of organic pollutants (wastewater treatment) have recently been developed by using supported iron and nickel nanoparticles (Mekki et al. 2021).

Still, a catalytic moist air oxidation system has been reported as a potential technique for treating organic contaminants in wastewater produced by different harmful and non-biodegradable sectors (Kumari and Saroha 2018). This approach has extensively treated numerous model pollutants, including; phenols, carboxylic acids, nitrogenous chemicals and other industrial effluents with various heterogeneous catalysts (Kumari and Saroha 2018). A report show that Fe-doped ZnO nanocatalysts were studied for degradation of the widely used medication amlodipine besylate from the environment (Alizadeh and Baseri 2018). Results indicate that the catalyst achieved higher degradation efficiency of amlodipine besylate of up to 90%. In another study, Cu-doped ZnO nanoparticle catalyst was investigated for its ability to degrade colours in wastewater (Shahpal et al. 2017). The substance was discovered to be a viable and promising catalyst for the non-photo degradation of dyes which are found in the wastewater generated by the printing and textile industries. Still, crystal violet, a synthetic organic dye was used to test the photocatalytic activity of cobalt-doped tin oxide nanoparticles (Sivakarthik et al. 2016). The results demonstrate that SnO_2 nanoparticles doped with cobalt are efficient photocatalysts for the decomposition of crystal violet. In this regard, these shreds of evidence reveal that catalysis is a critical phenomenon in conserving the environment, thus keeping it clean and safe for humankind.

Catalysis in the oil and gas industry

Catalysts emerged as one of the most potent instruments in the petroleum refining business during the last century (Emam 2013). In the modern world, producing green fuel oil is critical to preserving the environment and human health. Fuel oil that contains sulphur-containing compounds such as mercaptans, thiophenes, benzothiophenes and dibenzothiophenes, when burned, produces sulphur oxide, which is the primary cause of air pollution and acid rain (Emam 2013; Rezvani et al. 2018a, b; Rezvani et al. 2018a, b). Sulphur refractory compounds such as 4,6-dimethyl dibenzothiophene and other alkyl-substituted thiophene derivatives must be entirely and effectively removed from fuel oil to satisfy the new sulphur criteria (Chen and Li 2015; Hossain et al. 2019). Amidst alternative techniques for desulphurisation, the oxidative process has garnered significant interest as a potentially effective method because of its favourable reaction conditions of low temperature and pressure, increased selectivity in eliminating aromatic sulphur compounds and lack of costly hydrogen use (Abdelrahman et al. 2018; Betiha et al. 2018). As a workable substitute and addition to the hydrosulphurisation method, the oxidative desulphurisation method using various catalytic systems has developed, opening up novel opportunities in the refinery sectors. Because of the process's increased rate of removal of sulphur, thiophene derivatives have recently drawn increasing attention (Hossain et al. 2019). Besides, molybdenum oxide catalysts boosted with cobalt or nickel have been extensively utilised in the petroleum refining sector to hydrodesulphurisation of sulphur compounds (Segawa et al. 2000).

Other studies show that metal oxide catalysts are vital to most petrochemical and refining operations and important for enhancing environmental quality (Védrine 2017). Research suggests that using nanocatalysts have enhanced the efficacy of petrochemical and oil refining procedures (Peng et al. 2018). On the other hand, high-demand chemical commodities can be produced from methanol by using alternative feedstock like carbon dioxide, biomass, waste or natural gas via the intermediate formation of syngas (Yarulina et al. 2018). These products include ethylene and propylene (methanol-to-olefins), hydrocarbons (methanol-to-hydrocarbons), gasoline (methanol-to-gasoline) and aromatics (methanol-to-aromatics). This process has been the focus of research in academia and industry (Yarulina et al. 2018). Despite being discovered in the late 1970s, this catalytic technology has recently been applied industrially, with many sizable commercial plants currently up and running in Asia. Studies show that zeolite-based catalysis is applied in methanol-to-hydrocarbon processes (Martinez-Espin et al. 2017). Still, in the petroleum refining sector, clay catalysts have garnered much interest because of their application in the catalytic cracking process (Emam 2013). Thus, catalysis is critical in the oil gas industry, and it enables the release of recommended products in addition to the utilisation and production of renewable energy from simple molecules.

Catalysis in the pharmaceutical industry

The pharmaceutical business is becoming more and more dependent on catalysis. Still, environmentally friendly and cost-effective industrial processes are made possible by the crucial technology of catalysis. Chemical targets are growing more complex in medication development (Busacca et al. 2011). An active pharmaceutical ingredient today requires an average of 12 synthesis stages and an increasing number of alterations in the process. Industrial chemists look to catalysis to efficiently synthesise these intricate structures (Busacca et al. 2011). It is a challenging endeavour requiring the cooperation of several disciplines to produce a workable catalytic process for industrial sizes (Busacca et al. 2011). An excellent illustration of how catalysis affects society is the manufacturing of menthol, a substance frequently used in the pharmaceutical industry (Busacca et al. 2011). The market's need for menthol far outpaced the amount that could be found in natural sources, and additional uncertainties like bad weather and unstable international relations made it harder to maintain a consistent supply of the product. Research indicates that a method for producing synthetic menthol involves the asymmetric isomerisation of prochiral allylic amines, which is catalysed by rhodium. This industrial technique produces thousands of metric tons of synthetic menthol annually for the global market (Noyori 2003).

Another noteworthy instance of the power of catalysis is the commercialisation of Jacobsen's hydrolytic kinetic resolution reaction, which produces valuable chiral synthons in metric ton quantities, which are chiral building blocks for synthesising pharmacological drugs (Busacca et al. 2011). Metal catalysis holds considerable promise for improving the sustainability of pharmaceuticals by providing more direct access to single stereoisomeric products and quicker and more effective synthesis pathways (Hayler et al. 2018). Recent advancements in iron catalysis have created an environment conducive to investigating novel cross-coupling uses in pharmaceutical research (Piontek et al. 2018).

It is appealing to build new catalytic processes that use iron because of its inexpensive cost, plentiful supply, easy accessibility and extremely low toxicity (Piontek et al. 2018). Evidence from reports indicates that supported nickel nanoparticles catalyst has been used to produce primary, secondary, tertiary and N-methylamines,

offering the chance to produce numerous functionalised, structurally varied, linear and branched benzylic, heterocyclic medication derivatives at a lower cost (Liu et al. 2020a, b). Still, research has indicated that palladium nanoparticle catalysts exhibited significant catalytic activity for the pharmaceutical industry using cross-coupling reactions, an essential reaction for medicinal applications (Elazab 2019). Therefore, catalysis is inevitable in the pharmaceutical industry for the straightforward synthesis of drugs and derivatives through shorter production schemes.

History of combinatorial methodologies in chemistry

Over two centuries, Thomas Edson applied a high throughput technique to categorise a proper material for the production of a long-lasting light bulb filament (Tsapatsaris 2008). He created and tested thousands of different filaments to obtain one that could sustain for 1500 h and above; thus, the invention changed the application of electric light (Tsapatsaris 2008). A few years after, the father of combinatorial catalysis, Mittasch, created and tested 6500 catalysts in separate experiments in 36 months, assessing diverse combinations of substrates, catalysts, processing and conditions and produced the better form of the Haber–Bosch ammonia production pathway (McCullough et al. 2020; Newsam and Schuth 1999; Tsapatsaris 2008; Williams et al. 2019). In the Haber pathway assessed, the catalyst operates between 450 and 650 ℃ and an approximate pressure of 100 MPa while conversion of CO to CO_2 on locomotive catalysts, hydrocarbons to CO_2 and H_2O and reduction of nitrogen oxides works between 300 and 650 ℃ (Newsam and Schuth 1999). The methodological steps replicated from Mittasch's register are that catalysis evaluations need undertaking experiments with different elements under numerous combinations, screening at elevated pressure and temperature as in ammonia production in the Haber process, and a considerable number of screenings is needed (Tsapatsaris 2008).

However, in spite of the benefits of the invention of combinatorial technologies many years back, Mittasch's experimentations were time-consuming; thus, the invention of a new ammonia production catalyst came after a long period. As for drug discovery, combinatorial chemistry contributes to catalyst invention via pooled or parallel methods (Farrusseng 2008; Isbrandt et al. 2019; Newsam and Schuth 1999). Catalyst creation is one phase in a sequence that includes processing, accounting and catalytic screening, which constitute the term "High Throughput Experimentation" (Duff et al. 2004; Isbrandt et al. 2019; Newsam and Schuth 1999; Tsapatsaris 2008). High throughput experimentation in catalysis defines a logical formulation of an unending industrial style for condensed reactor dimensions, parallel screening and on-screen experimental control plus data management (Liu et al. 2022a, b; Rosen et al. 2019; Tsapatsaris 2008). Today, this technology is up and coming in terms of effectiveness via miniaturisation, computerisation, incorporation and the actual application of calculation (Isbrandt et al. 2019; Liu et al. 2022a, b; Newsam and Schuth 1999; Tsapatsaris 2008). The organisation and approach that facilitate high throughput catalytic material library invention are indicated in Fig. 1 (Turner et al. 2009; Volpe and Lugmair 2020).

The primary screening phase screens the combination of families of materials that could achieve a particular catalytic conversion. The phase is intended for the invention of "hits" which show promising material for a specific application (Liu et al. 2022a, b; Turner et al. 2009). For optimisation of data quality and mirroring the actual pathway conditions in primary testing, the quantity of experiments for acquiring excellent laboratory results is challenging (Turner et al. 2009). Primary testing provides qualitative styles in the results for the exclusion of a family of substances from a different library to classify the promising candidates as leads for screening in the secondary testing phase (Liu et al. 2022a, b; Turner et al. 2009). The candidate hits from the primary testing are evaluated in the secondary testing using at least precise technologies as conventional laboratory approaches (Liu et al. 2022a, b). Secondary testing techniques in heterogeneous catalysis facilitate that the identification of optimised leads suitable for the tertiary testing phase: scale-up and commercial screening in trial or semi-works establishments (Liu et al. 2022a, b; Turner et al. 2009).

Notwithstanding, combinatorial chemistry has attracted interest in diverse areas for many years. Using combinatorial chemistry for peptide production using solid resins was first reported by Merrifield in 1963 (Merrifield 1963). Since then, combinatorial techniques have progressed rapidly due to rapid technological development and computing (Isbrandt et al. 2019; Liu et al. 2022a, b). Therefore, technological advancement has resulted in the fast invention and optimisation of drugs and substances like super-conducting, ferroelectric, dielectric and luminescent materials along with ceramics, zeolites, organic substances and polymers, electrocatalysts, corrosion-resistant materials and heterogeneous catalysts (Aljohani et al. 2012; Emmanuel et al. 2019; Erdem and Yildirim et al. 2021; Guerin et al. 2006a, b, c; Isbrandt et al. 2019; Jandeleit et al. 1999; Mennen et al. 2019).

Hanak revealed a combinatorial technology in synthesising solid-state libraries of super-conducting substances in 1970 (Hanak 1970). A radio-frequency sputtering

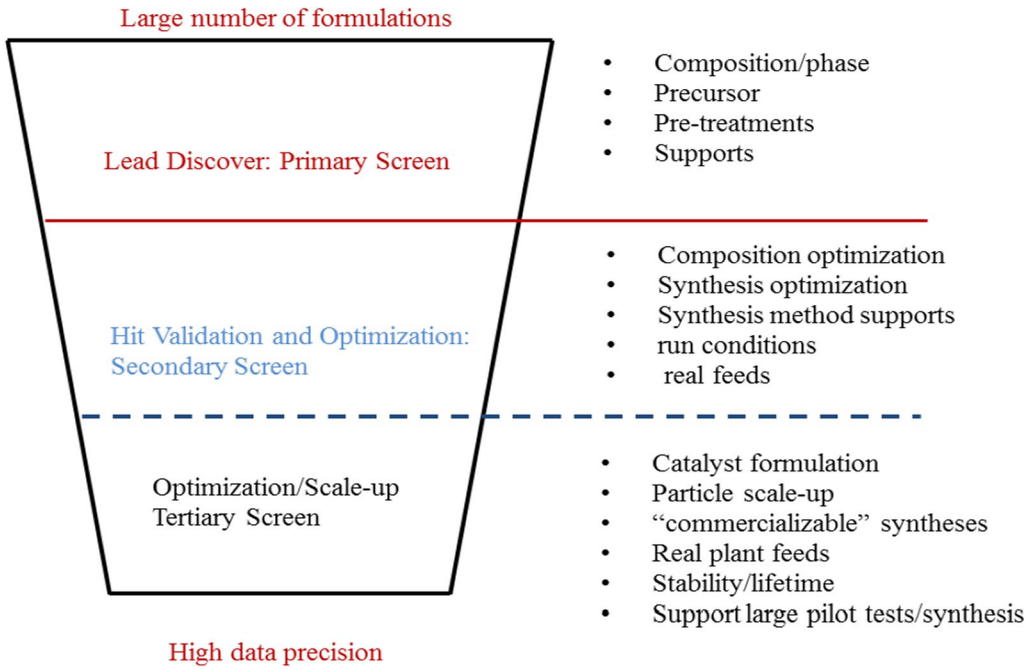

Fig. 1 Phases in the catalyst material library invention and optimisation indicating the parameters that are tested at every phase

technique was used to create binary or tertiary films with a linear alteration in configuration as the targets were placed at 180° for binary and 120° for tertiary films concerning the substrate (Hanak 1970). The technique led to a thirty-times rise in the rate of invention of materials (Hanak 1970). The use of sputtering via physical masking to deposit solid-state libraries for inventing and optimising CO conversion catalysts dates back two decades (Senkan 2001). In 1996, Moates et al. (1996) used a high throughput infrared thermography method to test combinatorial libraries of heterogeneous catalysts for hydrogen oxidation.

In 1999, Jandeleit et al. (1999) revealed a combinatorial technique used sequentially to create material libraries of noble metals catalysts for CO conversion and reduction of NO. Radio-frequency sputtering was applied to create materials via masks onto quartz materials of 75 mm diameter, attaining a triangular library which contained 120 catalysts synthesised in 60 min and then hardened at 773 K for 2 h to achieve alloy catalysts (Jandeleit et al. 1999). Scanning mass spectrometry was applied to test every catalyst through a direct selection of products through a capillary transmission line (Jandeleit et al. 1999). The drawbacks of a sequential masking method are that it is a time-inefficient approach requiring one to alter the masks position followed by a hardening phase to enable precursors mixing to attain the required materials. Studies show that the high throughput approach was applied to create a library of 66 Pt–Pd–In ternary catalysts using a tiny array and used a similar technique to test the dehydrogenation of cyclohexane to benzene (Liu et al. 2019; Senkan and Ozturk 1999). According to studies, different amorphous microporous mixed oxide-type catalysts were prepared using a high throughput combinatorial concept, and spatially resolved mass spectrometry was used to screen out the catalytic ability. The catalysts with copper showed high selectivity for the oxidation of propene with air (Liu et al. 2019).

High throughput technologies in heterogeneous catalysis

Approximately all high throughput catalyst testing is on large-area catalysts, which are somewhat unclear or undescribed (Hayden et al. 2007a, b). It is necessary to utilise the techniques with sufficient sensitivity on typical catalysts in which support and particle dimension are well managed and clear as previously attained in electrocatalysts (Hayden et al. 2007a, b). The function of the combinatorial approach in heterogeneous catalysis is critical in the current chemical industry as financial and ecological benefits are achieved through catalysts design and optimisation (Duff et al. 2004; Liu et al. 2022a, b). High throughput testing and material library creation methods are also important for rapid library creation and testing (Chan 2015; Liu et al. 2022a, b). For instance, the catalytic activity for exothermic reactions is easily tested by infrared thermography (IR), a method for heterogeneous catalyst libraries testing initially addressed by Moates

et al. (1996). This technique has been used to invent and establish a combination of oxides for low-temperature CO conversion (Saalfrank and Maier 2004). In the study, a combinatorial approach was used to create a library of 256 combinations of materials for effective low-temperature CO conversion and parallel activity testing was attained through an IR technique (Cypes et al. 2007), which provides qualitative or semi-quantitative results (Emmanuel et al. 2019).

In another study, a sequential impregnation technique anchored on robotic functionality was used to create a combination of catalytic materials on support from precursor substances (Hahndorf et al. 2002). Parallel testing of catalyst libraries was undertaken in a 64 multi-channel ceramic container linked with a rapid GC–MS examination (Hahndorf et al. 2002). Besides, an in situ resonance-enhanced multi-photon ionisation (REMPI) coordination with microelectrode recognition coupled with an array of micro-reactors for the invention of an optimal composition in ternary Pt/Pd/In metal catalysts for the dehydrogenation of cyclohexene into benzene has been described (Senkan and Ozturk 1999). Array micro-reactors facilitated parallel testing of vast amounts of catalysts at equivalent experimental settings. Designed multimetallic catalysts on a support were robotically created via an experimental co-impregnation approach where pellets of porous alumina were added into an aqueous solution of catalyst precursors at different concentrations (Senkan and Ozturk 1999). The pellets were dried at 90 ℃ for 4 h and further dried at 120 °C for an extra 4 h, and the impregnated pellet catalyst libraries containing 66 ternary blends of Pt, Pd and In were finally calcined at 500 °C for 2 h (Senkan and Ozturk 1999). In the implementation of high throughput experimentations, a high throughput workflow has been established to create and screen 10,000 substances for heterogeneous gas-phase conversion and alkene epoxidation (Duff et al. 2004).

High throughput technology for creating heterogeneous catalyst libraries addressed above includes covering part of a substrate during material creation (Jandeleit et al. 1999). Besides, the produced library is then exposed to extra action like drying and hardening. The creation of a combinatorial material library of this kind is time-consuming. Additionally, other high throughput testing approaches described are rather challenging. For example, REMPI is specifically used to test specific molecules, and many molecules do not contain REMPI characteristics. Mass spectrometry, which has broader applicability in gaseous mixture analysis, needs sample removal; thus, its use in combinatorial catalysis needs new methods. The quadruple mass spectrometry (QMS) method needs physical movement from one point to the other during catalyst material library testing. Thus, much time is used in the testing process. Principally, a combinatorial technique in heterogeneous catalysis needs the application of a sequential approach in catalyst material library creation and testing for required characteristics.

A high throughput method has been developed for solid–gas-phase conversion testing of heterogeneous catalysts centred on physical vapour deposition (HT-PVD) with the ability to concurrently create various material libraries (Guerin and Hayden 2006). The technique is combined with a high throughput material testing approach for testing created materials for specific properties. Since its discovery, the technique has been used in the creation of different material libraries (Aljohani et al. 2012; Emmanuel et al. 2019; Guerin et al. 2006a, b, c; Guerin et al. 2006a, b, c; Guerin et al. 2006a, b, c; Guerin et al. 2008). It creates combinatorial libraries with well-managed material composition ranges throughout the support and achieves sequential deposition of different elements (Guerin and Hayden 2006). The technique has enjoyed application in the creation of catalysts substrate and supported metal electrocatalysts (Guerin et al. 2006a, b, c; Guerin et al. 2006a, b, c; Hayden et al. 2007a, b; Hayden et al. 2009), hydrogen storage substances (Guerin et al. 2008), ternary metal alloy electrocatalysts (Guerin et al. 2006a, b, c), supported metal nanoparticles electrocatalysts (Guerin et al. 2006a, b, c) and corrosion-resistant thin-film alloys (Aljohani et al. 2012). More importantly, it has been used in the creation and invention of heterogeneous catalysts for solid–gas-phase, solid–liquid-phase reactions (Cypes et al. 2007; Hagemeyer et al. 2004; Holzwarth and Maier 2000) and in heterogeneous catalysts investigation (Emmanuel et al. 2019; Hagemeyer et al. 2004; Turner et al. 2009). Besides, a high throughput approach for material synthesis that integrates a rotatable "shadow" mask to create material libraries with a composition gradient through the substrate termed as rotatable shadow mask compositional spread alloy films (RSM-CSAF) deposition technique has also been reported (Fleutot et al. 2012). Still, Trapp reviewed the gas chromatographic high throughput screening techniques and applied various high throughput testing approaches in catalysis as key tools in the screening and discovering heterogeneous catalysts (Trapp 2008). Very recently, Emmanuel et al. (2019) applied HT-PVD coupled with a newly designed high throughput approach in testing well-managed supported typical heterogeneous nanoparticles catalyst by a high throughput infrared thermography method. The approach enables the evaluation of the particle size and substrate effects on typical heterogeneous catalysts. It has allowed the exploration of the particle size influence and activity of 100 supported gold nanoparticle catalysts for CO conversion at low temperatures.

The IR method is frequently useful in testing catalysts materials libraries because of its ease usability and is a parallel technique for testing heterogeneous catalysts activity (Moates et al. 1996; Senkan 2001). The strength of the infrared thermography approach in parallel testing of material libraries was addressed by Moates et al. (Moates et al. 1996), which was subsequently refined (Moates et al. 1996), including the emissivity variations of catalysts on the library, enabling the method to provide quantitative data (Holzwarth et al. 1998). It was applied to evaluate the activity of a combinatorial library of heterogeneous catalysts for the hydrogenation of 1-hexyne and oxidation of isooctane and toluene. Later, the emissivity-corrected infrared thermography (ecIRT) approach was used to test a heterogeneous catalyst library for toluene oxidation (Holzwarth and Maier 2000). The use of ecIR approach in inventing and optimising catalysts for hydrogen-rich gas cleansing by CO methanation was addressed (Krämer et al. 2007).

Consequently, it arose as a vital tool in the testing and inventing heterogeneous catalysts, catalysis investigations and investigations of catalyst potentials and characteristics. The approach has been used in the invention and establishment of a combination of oxides catalysts for low-temperature CO conversion (Emmanuel et al. 2019; Saalfrank and Maier 2004), the invention of effective catalysts for low-temperature CO oxidation (Cypes et al. 2007), investigation of the dehydrogenation process of cyclohexene over carbon-supported Pt catalysts (Biniwale et al. 2005) and study oscillatory behaviour in the course of catalytic oxidation of CO over supported Pd (Digilov et al. 2004). It has also been applied in testing of hydrogen storage materials (Domènech-Ferrer et al. 2011; Guerin et al. 2008), in high throughput investigation for the invention of catalysts for solid–gas-phase, solid–liquid phase reactions (Biniwalea et al. 2005; Cypes et al. 2007; Krämer et al. 2007; Loskyll et al. 2012; Moates et al. 1996; Saalfrank and Maier 2004; Scheidtmann et al. 2001) and endothermic dehydrogenation reactions (Biniwalea et al. 2005).

In the same vain, the ecIRT approach was reported as a potent tool in catalysis research (Emmanuel et al. 2019; Loskyll et al. 2012). It is a useful tool in primary testing for anticipation of targeted characteristics of interest needed for qualitative catalyst identification, for example, simply assessment of catalytic activity instead of structure and other characteristics leading to unnecessary data during the discovery stage; thus, fast parallel catalysts testing techniques are required for rapid parallel data acquisition from the catalyst libraries and saving analysis time (Scheidtmann et al. 2001).

The catalytic activity of dry methane reforming by high throughput screening technique in order to formulate alloy catalysts which are stable, highly active and less expensive has been studied (Yu et al. 2021). Alloys made of 39 elements were screened for the dry methane reforming catalyst, where 23 binary intermetallic compounds were found to be likely catalysts (Yu et al. 2021). In another study, the high throughput technique was used to produce RuO_2-graphene heterogeneous catalysts using a hydrodynamic route for selective alcohol oxidation (Jeong et al. 2018). A high throughput system for the creation and simultaneous testing of up to 96 heterogeneous catalysts has been recently developed, which portrays a scheme for rapid testing of different species of mesoporous metal oxide catalysts for the oxidation of morin (Potgieter et al. 2021). Sugiyama et al. (2021) applied deep learning and high throughput approaches in the direct formulation of heterogeneous catalysts in the oxidative coupling of methane reactions. The technique anticipated 20 catalysts from a 12,708 library, and the results showed that 9 of the anticipated 20 catalysts have not been recounted earlier (Sugiyama et al. 2021). Still, high throughput testing of heterogeneous catalysts for conversion of atmospheric nitrogen to ammonia has been recently undertaken by Choutipalli et al. (Choutipalli et al. 2022).

In the study, tantalum-based small metal clusters were tested for nitrogen reduction reaction (NRR) activities by computational techniques, and the findings show that out of forty-nine possible sites in eighteen metal clusters for nitrogen adsorption, only four sites (four clusters) were systematically anticipated which were highly promising catalysts for nitrogen reduction (Choutipalli et al. 2022). In a different study, Xue et al. (2021) conducted a high throughput testing of a transition metal single-atom catalyst supported on a C_9N_4 substrate for nitrogen reduction reaction using the first-principles density functional theory calculations. In the study, 24 candidates were screened for N_2 reduction activity. Only one candidate showed a good response for N_2 reduction, which possesses high promise for experimental production because of its greater thermodynamic strength (Xue et al. 2021).

A low-cost combinatorial technique for evaluation of an array of metal oxide materials as photocatalysts for solar fuel generation using spray pyrolysis has also been reported very recently, which allowed the synthesis of four metals three-at-a-time triangular patterns to screen a compositional array of promising photocatalysts (Compton et al. 2019). Through this technique, a sodium-doped copper bismuth oxide photocatalyst has been discovered and soptimised (Compton et al. 2019). In another study, a high throughput approach was applied to create and test high-performance ansa-zirconocene olefin polymerisation catalysts (Ehm et al. 2020). A high throughput technique based on periodic density functional theory

has been developed, which screens huge numbers of metal–organic structures for promising catalytic candidates in which the partial oxidation of methane was considered to identify the promising catalysts (Rosen et al. 2019).

Nevertheless, Liu et al. (2022a, b) addressed the key processes of high throughput technologies for the synthesis of catalyst libraries containing the virtual laboratory creation anchored on informatics tools and experimental data laboratory, including the formulation of experiments, reactants created manually or automatically, construction of reactor to control the variations like materials differences and reaction environments and parallel characterisation of created catalysts. The achievement of high throughput synthesis requires the stage to perform a combination of experiments in less time and allows the effective management of reaction parameters (Liu et al. 2022a, b). Reports show that different production techniques are in place for high throughput examination, such as instrumental-enabled thin-film deposition techniques, physical and chemical deposition approaches and solution-based chemical reaction techniques (Liu et al. 2022a, b; Senkan and Ozturk 1999).

Several deposition techniques have been used in the synthesis of catalysts, like physical vapour deposition, plasma/magnetron sputtering, spray pyrolysis, chemical vapour deposition and electrodeposition, and provide an active path to create and dope films with any element (Compton et al. 2019; Guerin and Hayden 2006; Liu et al. 2022a, b). Solution-based techniques like impregnation, precipitation and sol–gel production, particularly for catalyst powders, have been established and used over the years, providing the advantages of controlling the materials' characteristics and flexibility in material compositions. For instance, the inclusion of dopants and these have been established to create different materials in a huge parameter space efficiently (Compton et al. 2019; Liu et al. 2022a, b).

According to studies, a mechanistic hypothesis may be an effective starting point for high throughput reaction development (Isbrandt et al. 2019). Reports show that organo-halides and aldehydes are intermolecularly coupled to generate ketones through a formal C–H bond functionalisation despite prior attempts to change this process into intramolecular or activated aldehydes reactions failing. In this investigation, reaction screens were carried out on the parameters considered the highest value, including 32 ligands, four bases, four solvents and eight pseudo-halides with Pd or Ni catalysts (Isbrandt et al. 2019). Utilising literature precedent to inform the experimental design, a non-exhaustive screen was conducted utilising 672 of the 8192 potential combinations. Only Ni catalysts should be investigated with the majority of pseudo-halide coupling partners due to Pd's inability to contribute to strong C–O bonds oxidatively. While the majority of trials produced no identifiable product, up to 8% yield was achieved using the Ni catalyst, multidentate phosphine ligand, weak organic base and organo-triflate substrate conditions that have been proven to be successful in Ni-catalysed Heck reactions in the past. This low-key beginning allowed for a more conventional OVAT optimisation, which produced very efficient conditions. Notably, any divergence from these characteristics, such as using Pd catalysis, organo-bromides, monodentate phosphines or inorganic bases, had no effect. This shows the significance of high throughput experimentation in enabling simultaneous screening of numerous variables to uncover hits that would be missed with OVAT techniques (Isbrandt et al. 2019). Besides, small Au and Pt nanoparticles have undergone extensive research for CO oxidation at low temperatures (Emmanuel 2022a, b; Emmanuel and Hayden 2022; Emmanuel et al. 2019; McCullough et al. 2020). High throughput IRT is an appealing way to screen several catalysts for this reaction simultaneously.

To assess the impact of their particle size on CO oxidation and to further clarify the process of CO oxidation utilising data from 100 distinct Au or Pt/TiO_2 catalysts, parallel IRT has been used to measure CO oxidation over a series of amorphous titania supported Au and Pt catalysts (Emmanuel and Hayden 2022; Emmanuel et al. 2019; McCullough et al. 2020). Changing the total flux of Au and Pt allowed for the deposition of Au and Pt particles of varying sizes onto TiO_2 thin films by using a high throughput physical vapour deposition technique, resulting in thin films of different thicknesses (Emmanuel and Hayden 2022; Emmanuel et al. 2019; McCullough et al. 2020). When screening was done, it was discovered that the TOF as a function of mean particle size was highest for the more petite Au and Pt particles and monotonically decreased as the particle size rose. This demonstrates the efficacy of several high throughput approaches to explore the intricate connections between synthesis factors, promoter components, catalyst characteristics and catalytic activity towards discovering and improving novel catalytic materials.

In another study, using a high throughput continuous hydrothermal flow synthesis system, a library of 66 perovskite $Ba_xSr_yCa_zTiO_3$ samples of catalysts was made in just 14 h. The samples were then collected from the process's outlet, cleaned and freeze-dried before being tested individually for oxygen reduction using a rotating disc electrode testing method. The method was proven effective at quickly identifying oxygen reduction catalysts from new libraries of electrochemical materials (Groves et al. 2020). Additionally, because of the synergistic

effects of the elements, multicomponent alloys are attractive candidates as catalysts for the hydrogen evolution reaction in aqueous solutions, although the challenge is to find the best catalyst. The best compositions with advanced intrinsic catalytic activities in alloys combination of Ni–Co–Ti and Ni–Fe–Au have been identified using a high throughput bubble screening method, which demonstrated the ability to identify the multicomponent alloys with the highest catalytic properties (Liu et al. 2022b). It has been stated that this approach is unlimited to ternary catalysts for hydrogen evolution reactions, but it is also anticipated to be equally beneficial for researching catalysts in higher composition alloy systems and even for oxygen evolution reactions and Ni–Fe–Au (Liu et al. 2022b).

A high throughput technique has been used to synthesise and screen multimetallic cluster catalysts on carbon support for oxygen reduction reaction (Yao et al. 2020). The catalyst was synthesised by formulation in solution followed by rapid thermal shock of precursors to allow alloy creation. Adding one element at a time produced various multimetallic clusters ranging from ternary, PtPdRh to octonary, PtPdRhRuIrFeCoNi materials. The two top-performing catalysts for the electrochemical oxygen reduction reaction were swiftly identified by employing scanning droplet cell analysis to quickly screen the compositionally diverse multimetallic clusters with similar size and structure. The performance of the improved multimetallic catalysts was assessed in a representative rotating disc setting and contrasted with that of a Pt control sample. The rapid synthesis and compositional study of multimetallic as improved catalytic materials are thus made possible by the combinatorial and high throughput technique (Yao et al. 2020). According to studies, a hierarchical high throughput catalysis screening technique has been created to improve catalysts for synthesising ammonia. The new leads have undergone comprehensive mechanistic tests for validation (Fuller et al. 2022). Studies show that the high throughput method of catalytic olefin polymerisation has been thoroughly assessed in terms of its ability to create new materials and large, accurate databases for the analysis of quantitative structure–property relationships for the olefin blocks copolymers generated under chain-shuttling polymerisation. The breadth of the polymer expertise and usefulness chains this strategy covers, from catalytic synthesis through engineering, is unique. (Ehm et al. 2020). The procedure might be used as a model for high throughput manufacturing and analysis of novel materials, reducing the time it takes for new goods to hit the market. The study's findings also show how reliable the approach is.

In the field of materials science, the application of statistical and machine learning techniques has grown in popularity recently (Baumes et al. 2004; Li et al. 2017; Vasudevan et al. 2019; Palkovits and Palkovits 2019; Li et al. 2017). When applied properly, artificial intelligence (AI) has the potential to revolutionise not only the speed at which scientific discoveries are made but also the methodology of materials science. It is a unique approach to finding new materials that has been reported, and combines machine learning algorithms with experimental high throughput catalytic data and elemental properties. It predicts future catalyst performance and directs synthesis using a modest experimental data set and chemically descriptive characteristics (Erdem and Yıldırım 2021; McCullough et al. 2020; Williams et al. 2019). This led to the identification of several novel ammonia breakdown catalyst compositions, which were experimentally tested in comparison to recent ammonia decomposition catalysts and were found to have remarkable low-temperature performance at far lower weight loadings of Ru. Besides, a comprehensive machine learning approach using descriptor-based kinetic analysis to quickly screen bimetallic catalysts has been reported in an effort to find bimetallic catalysts more quickly (Li et al. 2017). This method can quickly filter down potential candidates for specific applications and explore a large chemical space with tremendous compositional and configurational degrees of freedom. Still, using the existing data sets from the literature, combinatorial heterogeneous catalysis and machine learning techniques have been applied to predict water oxidation catalysts (Palkovits and Palkovits 2019). Based on the given data sets, the machine learning models provide a respectable prediction precision, demonstrating that even basic models may produce accurate projections. Though machine learning is becoming more and more popular across a range of fields, its use in catalysis is still in its infancy (Yang et al. 2020), thus subject to more research and realisation.

Besides, the growth and progress of high throughput systems in catalysis that have been discussed herein, the methodology is currently being used in its entirety for commercial purposes, and research attempts are still ongoing to connect the method with artificial intelligence. High throughput technologies are nearly being integrated into industry gradually and have had significant positive economic effects. For instance, Symyx Corporation produced fresh heterogeneous catalysts (Liu et al. 2019). Studies of the catalytic chemical, petroleum, biochemical and environmental technology that were successfully marketed during the decade of the 1990s provide over 130 instances of new catalysts or catalyst modifications for operational processes. These procedures are either already commercialised or are in an advanced upscaling phase (Armor 2001). Besides, the creation of Nebula

catalysts, which ExxonMobil jointly developed with Albemarle Catalysts, represents a significant advancement in hydrodesulphurisation catalyst technology (Kerby et al. 2005). Nebula's activity is at least three times more than earlier hydroprocessing catalysts. It is now commercially available for several uses, such as distillate hydrocracking and ultra-low sulphur diesel fuels. The creation and commercialisation of a new catalyst for the hydrodesulphurisation of gasoline distillates that has 30% more activity for sulphur removal and 50% more selectivity than the currently used commercial catalyst have demonstrated the viability of a workflow that enables rapid, effective heterogeneous catalyst discovering and improvement (Turner et al. 2009).

Challenges facing high throughput technologies and future outlook

Shreds of evidence show that high throughput techniques have excellent properties, and critical attainments are in place. However, there are challenges which require solutions, including the technique is not fully realised in industry and academia, the existence of few facilities featuring the state-of-the-art automated catalyst fabrication stage, detailed knowledge of the microstructure of the catalyst through high throughput screening techniques either on situ or online, few practical and smart data visualisation tools for capturing detailed correlations, trends and patterns within massive data, existing gap among high throughput computational and experimental screening technologies and the absence of databases for combination of high throughput computational and experimental analysis enriched with diverse information on parameters. The answer to these challenges would provide an in-depth knowledge of the catalysis scheme and promptly fasten the catalysts discovery process.

However, the literature reveals the promise of high throughput technique in catalysis. The full realisation of a computerised laboratory and the informatics tools for massive data handling during the investigation of particular material characteristics is critical. There is much enthusiasm towards this new technology, which enables fast development of heterogeneous catalysts in academia and industry. Emphasis is on automated approaches based on robotics or materials-dispensing machines coupled with high throughput characterisation systems for fast learning of the synthesised catalytic material libraries' performance to fasten catalyst discovery. More researches are required on the application of combinatorial high throughput methodologies with artificial intelligent.

Conclusions

Catalysis is a significant phenomenon in academia and industry that has grown significantly over years. It is crucial in many sectors, including production, pharmaceutical, chemical and energy industries, and environmental conservation. Besides, high throughput experimentation is key and widely used in material sciences. The technique has demonstrated its high effectiveness, cost-cutting and low running time characteristics, resulting in fast discovery, synthesis, screening and optimisation of catalysts. The technique is growing sufficiently in academia and industry. It responds to a question of the low effectiveness of the previous traditional method of catalyst invention based on studying only one composition at a time. A wide range of literature reveals significant progress in using high throughput technologies to invent catalysts involving designing, synthesis and screening.

Abbreviations

BASF	Badische Anilin-und Sodafabrik
AI	Artificial intelligence
CO	Carbon monoxide
CO_2	Carbon dioxide
ecIRT	Emissivity correction infrared thermography
GC-MS	Gas chromatography mass spectroscope
HT-PVD	High throughput physical vapour deposition
IR	Infrared
IRT	Infrared thermography
REMPI	Resonance-enhanced multi-photon ionisation
RCA	Radio Corporation of America
RSM-CSAF	Rotatable shadow mask compositional spread alloy films
NO	Nitrogen monoxide
OVAT	One variable at a time
USD	United States Dollar
QMS	Quadruple mass spectrometry

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