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Prof. Dr. Hannes Utikal

20 years of the Journal of Business Chemistry: The academic journal for management issues in the chemical and pharmaceutical industries

Uday Grover, Janvee Garg and Prof. Anil Kumar Singh

From brass to brilliance: Frugal innovation for safer public spaces

Dr. Steffen Kanzler

A conversation about artificial intelligence at Evonik

Dr. Andreas Konrad

How artificial intelligence can be used in the chemical industry

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Aim and Scope

The Journal of Business Chemistry (JoBC) focuses on current developments and insights at the intersection of management and chemistry, biotechnology or pharmacy.

The JoBC provides an international forum for researchers and practitioners in companies, research institutes, public authorities, consultancies or NGOs to present and discuss current challenges as well as potential solutions in an interdisciplinary manner. Thus, the JoBC aims to foster the dialog between science and business, to support management practice in the chemical and pharmaceutical industry and to indicate where further research from academia is needed. The JoBC offers high quality publications with academic standards, a fast publishing process and global reach. With this multidisciplinary and boundary-spanning approach, the JoBC intends to become the leading journal for decision makers in the chemical and pharmaceutical industry.

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Letter from the Editor

- 20th anniversary of the Journal of Business Chemistry -

Dear Readers,

This year we are completing 20 years of publishing our journal, the first of which was published in May 2004, edited by Dr. Stefan Picker, Dr. Carsten Vehring and Prof. Dr. Jens Leker. Since then, 59 issues including 85 research papers, over 80 articles within the practitioner's section and 54 commentaries have been published in order to inform the business chemistry community about new insights in research and in practice. Looking back we are grateful for the support of our readers, authors, and reviewers over the years, and we look forward to continuing to provide insightful and informative articles on management issues in the chemical industry.

This June 2024 issue comes with a novelty, we are introducing a new category of articles: interviews with experts in the field of chemistry and management. For this issue we have conducted two interviews, one with Prof. Dr. Hannes Utikal from the Provadis Applied University in Frankfurt and one with Dr. Steffen Kanzler, Marketing Director at Evonik. This new category of articles in our journal intends to get even closer insights from challenges at the intersection of chemistry and management, both in academia and practice. Furthermore, the key themes of this issues are reflections on the history of our journal, the concept of frugal innovation, current trends and the application of artificial intelligence (AI) in the chemical industry.

In the interview with Prof. Utikal: "20 years of the Journal of Business Chemistry – the academic journal for management issues in the chemical and pharmaceutical industries!" he reflects on the many years that this journal has been published, how the journal has evolved with time and influenced theory as well as practice. He also introduces the Zentrum für Industrie und Nachhaltigkeit at the Provadis Hochschule.

The research paper in our June issue "From brass to brilliance: a frugal innovation for safer public spaces" by the authors Prof. Anil Kumar Singh, Janvee Garg and Uday Grover explores the use of brass as an affordable and effective solution to improve public sanitation in high-traffic public health settings, like hospitals and public transport systems. The study is based on the principles of frugal innovation, which prioritize resource efficiency, affordability, accessibility, and sustainability. It evaluates the effectiveness and economic feasibility of various brass applications for microbial control on high-touch surfaces. The study finds that brass applications not only reduce the need for frequent sanitation but also offer durability and long-term effectiveness in public spaces. Incorporating brass into public infrastructure significantly reduces infection rates and healthcare costs, aligning with the frugal innovation approach of maximizing value with minimal resources. The study contributes to public health strategies by highlighting the role of brass in sustainable and economically advantageous solutions.

In the interview with Dr. Steffen Kanzler we discussed current topics and trends in the chemical industry as well as applications of AI at Evonik and its potential for future use cases. Getting this first-hand knowledge from examples at Evonik gives us an interesting point of view and introduces us to the next article from Dr. Andreas Konrad.

Dr. Andreas Konrad contributed with an article on current and potential future applications of AI in the chemical industry. In his article „How artificial Intelligence can be used in the chemical industry“ he particularly focuses on safety and accident prevention, innovation, R&D, supply chain optimization and tools to improve the customer experience, he also mentions risks and concerns regarding the application of AI in chemical companies.

Please enjoy reading the second issue of this year, we are grateful for the support of all authors and reviewers for this insightful issue. If you have any comments or suggestions, please do not hesitate to contact us at contact@businesschemistry.org for more updates and insights on management issues in the chemical industry, follow us on LinkedIn: www.linkedin.com/company/jobc/ and subscribe to our newsletter.

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Interview

with Prof. Dr. Hannes Utikal*

Combining perspectives: How we are creating impact.

20 years of the Journal of Business Chemistry: The academic journal for management issues in the chemical and pharmaceutical industries

When you reflect about your many years of experience publishing the Journal of Business Chemistry, what key insights or lessons have you gained about the intersection of the chemical industry and economics?

The chemical industry is a fascinating industry characterized by some specifics at the intersection of natural science and management theory:

The chemical and pharmaceutical industries are energy- and capital-intensive **process industries** - still largely based on **fossil fuels and feedstock**. These industries encompass thousands of products used in different applications and enabling innovations on the side of their customers ("**industry of industries**"). The industry consists out of different segments, each having specific success factors, and typically showing a multiregional character. The industry has a long tradition, with the initial years of industrial chemical industries being dated back to the 1860s in Great Britain. Applying insights from industry lifecycle theory, the industry seemed to be until the 2010s in its maturity phase where the basic technological know-how is well diffused, and the focus is – except for patent-oriented pharmaceuticals and some innovative specialty chemicals – more on the side of technological improvements than on the side of breakthrough innovations. But with the need to defossilize its energy and feedstock base, the industry is currently confronted with the **need to reinvent itself**, its energy base, its feedstock, its value proposition to customers and society and the main technologies.

In addition, advances in biotechnology offer new opportunities for individualized pharmaceutical treatments and production processes, too. And advances in digitalization allow for product and process innovation. **Societal expectations** towards the reductions of the negative social and environmental impact of the chemical and pharmaceutical industries have been increasing over the years. **Geopolitical tensions** and international differences in environmental and social regulations influence the global footprint of the chemical and pharmaceutical industries, too. This is especially true for the 2020s.

These industry characteristics are an eldorado for researchers from the fields of chemistry, engineering and management theory: What **dynamic capabilities** do companies in the chemical industry need to master the described challenges? How will the **transition to a climate-neutral industry** be financed? What is the most promising public financial support mechanism to avoid carbon leakage and foster green innovation? What are successful **sustainable business models**, allowing for positive economic, ecological and social impact? What are relevant regulatory developments for supporting green and sustainable finance? How will the **global footprint of value activities** change due to regulation and geo-political developments? And how will managers handle the ambiguities in the transformation phase with tensions between different economic goals and time horizons?

All these aspects can only be meaningfully approached with a profound understanding of the industry specifics and with the will to integrate research methods and findings from natural and social sciences.

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Is there anything that has changed in recent years and are there examples where the journal influenced the industry practices?

The Journal of Business Chemistry has been a platform for the reflection upon current developments in the different segments of the chemical and pharmaceutical industries. Important topics for the chemical industry in the period 2000-2024 were

- **Decarbonization and sustainability**: The chemical industry is in the focus of climate policy and must significantly reduce its greenhouse gas emissions. The advances of the industry are largely interconnected with the activities of other stakeholders providing access to green energy and feedstock, regulate carbon capture and storage (CCS) and deciding about the regulatory and financial framework. Success of the Industry thus requires successful stakeholder management with a variety of private and public stakeholders.
- **Rising production costs and falling demand**: The chemical industry in Europe is struggling with high energy prices, inflation and falling demand. This is having a negative impact on competitiveness, particularly in energy-intensive sectors such as basic chemicals. The question of the future allocation of value chain activities is of utmost importance to European jobs and wealth.
- **Digitalization and technological change**: New technologies such as AI and data analysis offer the chemical industry opportunities to increase efficiency and innovate. The industry must adapt to the digital transformation, identify new business models and optimize its production and innovation processes.
- **Global shifts**: Asia, especially China, continues to gain importance as a production location for chemicals. European and American manufacturers must increase their competitiveness. This holds true as well for industrial parks – a trend towards the globalization of industrial park management competencies can be observed in recent years.
- **Skills shortage**: Demographic change and an ageing workforce pose challenges for the chemical industry in Europe in terms of recruiting and retaining staff. The workforce will become more diverse with regards to its skills and backgrounds, increasing leadership challenges.

These topics have been addressed in the Journal of Business Chemistry, too.

In 2023, we had a **special issue** on the topics of the **transformation of the European process industries towards climate-neutrality**, covering a broad range of important topics from different fields of natural and social sciences. In 2020 we published another special issue focusing on recent developments in the **innovation and production management in the process industries**. These special issues highlighted in a condensed manner the relevant questions of that time. They were developed in conjunction with academic workshops initiated by Professor Dr. Dr. Thomas Lager, Malardaren University, Sweden.

I appreciate the different types of articles we publish in the Journal of Business Chemistry: The **research articles** highlight innovation and original findings from research. The **practitioners' section** gives the floor to practitioners' sharing their experiences in form of a case study. This is especially valuable as a lot of the above-mentioned challenges are observed firsthand in management practice: Framing these challenges and reflecting upon those is an important value add of our journal: As James March has put it: "No new organizational forms have been invented by academics, they are invented by practitioners having to deal with specific challenges". The same holds true for the management challenges in the chemical and pharmaceutical industries. Being **close to the real-life challenges** allows to identify them and make them ready for academic investigation. Bridging the **gap between academia and practice** is one of the strengths of the journal. And the **commentary** is a forum for sharing substantial arguments on recent developments at the intersection of business and chemistry – these are a forum for sharing practical experiences and theoretical reflections in an early stage to foster the discourse on management challenges in the chemical and pharmaceutical industry.

As the editor of a long-standing journal on Business Chemistry, how do you see the role of interdisciplinary research in advancing sustainable practices within the chemical industry, and what advice would you offer to young researchers interested in this field?

I strongly believe that a practically relevant topic should be at the center of a research endeavor at the intersection of natural sciences and social sciences. Let's focus on the interface of industry specifics and management theory to create impactful research!

Once a "relevant" question is identified, the methodological questions need to be addressed (gathering and analyzing data etc). Of course, this implies the methodological rigor of the respective discipline, either in natural or in social sciences.

At the same time, it is crucial that the researcher has a profound understanding of the **multidimensionality of the practical problem**. For example: Changing from a combustion engine to a battery-based engine, does not solve all mobility challenges we face in cities (e.g. traffic jams). Often technical product innovations need to be accompanied by process and social innovations too (e.g. alternative ways of guiding traffic, changing mobility preferences). Thus, the researcher needs to see the field where she or he can make the scientific contributions – but needs to see the **embeddedness of the research activities in the broader societal developments**. Identifying and managing these linkages to the broader societal context, engaging in an inclusive language what can be understood by members of other societal groups too, is the prerequisite for **creating a societal impact**, if desired.

Being based at an industrial park, I see a broad range of highly practically relevant research questions and propose to capture some of them through **in-depth case study research**. I always like to bridge the gap between practice and academia. At the same time, I'm fully aware that some academic journals do not value case studies as they do prefer large scale quantitative research. Young researchers should be aware of their target – where do they want to create an impact and where do they see their future careers – and should choose the research setting accordingly. But I would be skeptical if a research question would only be selected due to the availability of a large scale-dataset allowing for elaborated statistical analysis but lacking practical relevance. **Young researchers need both: Practical relevance and scientific rigor**. Just one of these aspects is not enough.

In addition, I'm convinced that management issues in the **chemical and pharmaceutical industries are "under-researched"** – given their high societal, economic and ecological impact. As "the industry of industries" providing the basics for the majority of physical products and with high direct and indirect effects on planet and people, I believe that the scientific community has still the potential for **creating a shared understanding of the most pressing issues** with relevance for the industry at the intersection of natural and social sciences. While the research questions in the field of chemistry as natural science are not context specific ("we need green and sustainable chemistry") I miss a shared research agenda for the management challenges in the chemical and pharmaceutical industries **highlighting the context of different continents and countries**. The natural, regulatory, political, social and economic environment influences management decisions in different countries. Analyzing this context and qualifying young researchers and students for acting context-specific, will advance the management of global chemical and pharmaceutical companies further. This will reduce he probability of developing isolated solutions (e.g. regulation on plastic in one region) at the expense of other regions (exporting plastic waste). **Systemic thinking and acting are needed for the "industry of industries"**, too.

You are also the head of the Zentrum für Industrie und Nachhaltigkeit at the Provadis Hochschule can you tell us a bit about this center? What are key projects of you in this regard and where can interested individuals find out more?

The Center for Industry and sustainability is located at the industrial park Höchst. For more than 150 years, industrial park Höchst has been a symbol of innovation and change. But how do you design a sustainable industry? We see ourselves as a **"think- and do tank" for a sustainable, future-proof industry**. We develop new knowledge, organize knowledge cycles and create a platform for knowledge exchange.

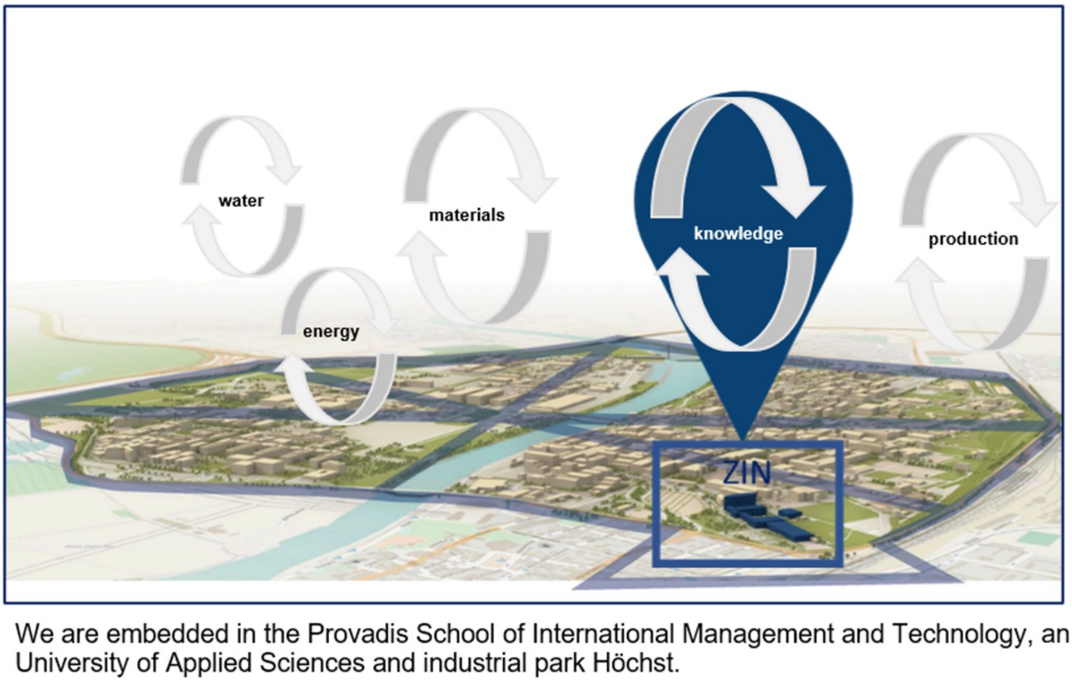

Figure 1 Location of the Provadis School of International Management and Technology in the industrial park Höchst (own representation).

In our innovative research and education projects, we develop practical solutions for the sustainable development of companies. We empower people to integrate sustainability into their business strategy and to transform their organizations. However, to achieve profound change and address the major challenges of our time, such as climate change, a supportive ecosystem is required.

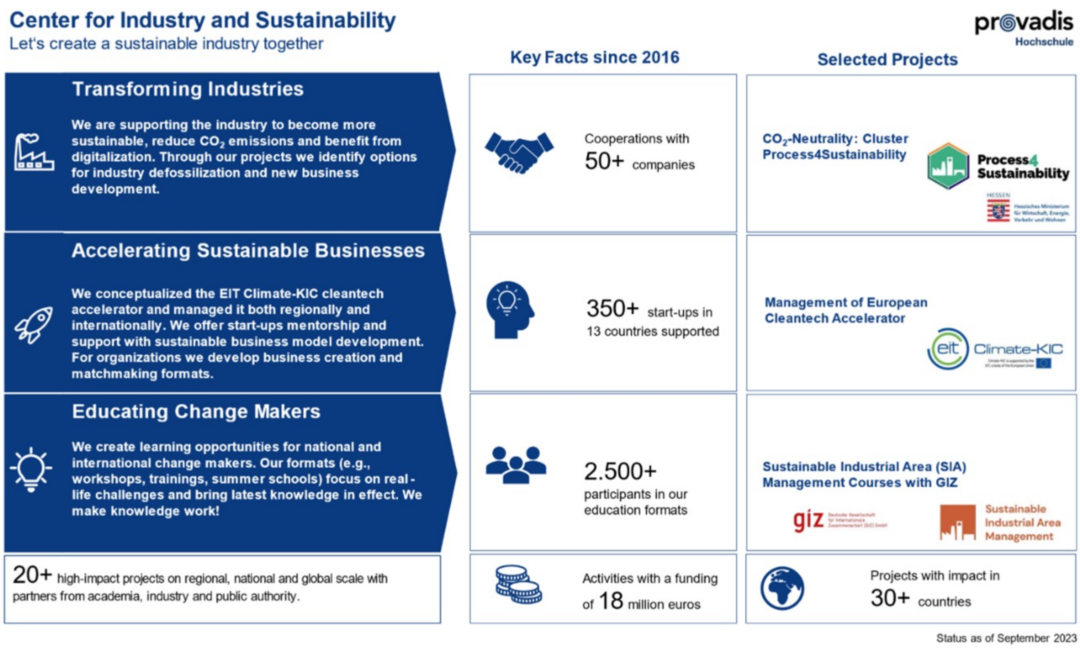

Figure 2 Overview of projects and key facts of the Provadis School of International Management and Technology (own representation).

With the vision of a CO_2-neutral process industry in Hessen, we founded the Process4Sustainability cluster with companies at industrial park Höchst. We believe that a sustainable industry can only be achieved by working together, which is why our activities are based on close cooperation with national and international partners from science, business, and the public sector. Therefore, in addition to companies, research institutes and social innovation partners are also part of our cluster. Further information about our cluster can be found here www.process4sustainability.eu.

In your opinion, what are some of the most pressing sustainability challenges currently facing the chemical industry, and how can academia and industry collaborate to address these challenges effectively?

Companies in the chemical and pharmaceutical industries are particularly challenged when it comes to their sustainable development. Let's take the transformation towards climate-neutrality as an example. We may differentiate between two interrelated challenges, which only can be solved when a variety of actors from all parts of society collaborate.

On the one hand, the transformation process must be handled from a technological and economic perspective:

- From a technological perspective, incremental technological changes are not enough to achieve climate neutrality; new technologies are required. For example, water electrolysis using renewable electricity to produce hydrogen, carbon capture and storage or the electrification of high-temperature crackers are being developed and tested. It is still difficult to estimate when which technology will actually be available on a large industrial scale and at what price. Large quantities of renewable electricity are a prerequisite for many alternative technologies. It is still partly unclear where, under what conditions and at what price green electricity will be produced. The ecological transformation of the chemical industry therefore also requires a cross-sectoral approach, which must take into account new national and international infrastructures to be established.
- From an economic perspective, many technologies for a defossilized chemical industry will not be competitive with conventional technologies due to their higher production costs without a global CO_2 price. The production costs are largely dependent on the development of the price of electricity and CO_2. Studies estimate the investment costs to be acceptable for society as a whole, but a challenge for individual companies. Against the backdrop of uncertain future framework conditions, companies assess whether and how they should change their business model and which technologies they should invest in. They not only have to plan how to enter new technologies (entrepreneurial innovation), but also how to exit established technologies (entrepreneurial exnovation). All of these decisions are highly dependent on the chosen regulatory framework. The transformation is thus not only dependent on technological and economic developments but as well on societal ones.

The **transformation process can be understood as a multi-actor decision-making process** with a variety of goals as many players bring very different perspectives to the solution of this challenge. If the transformation of the chemical industry is understood as a **decision-making problem** in which the best solution must be selected from a range of alternatives against the background of a target function, then the conflicts can relate to various elements of the decision-making model:

- Who constructs the **decision problem**? (A national government? The company? NGOs? Who with what legitimacy?)
- Which **alternatives** are considered? (Which technologies and policy instruments are taken into account?)
- Which **objectives** are used for the assessment and how are they weighted? (How are the various economic, ecological and social objectives to be weighted? Is the goal of 1.5 or 2 degree compatibility the leitmotif?)
- Which **benefit function** is assumed? (What is the environmental effect of which technology? What costs and benefits are incurred by companies or society? What impact do the decisions have on competitiveness and jobs in Europe?)
- How should the **timing of the decisions** be organized? (At what point in time should which decisions be made? Does it make sense for a company to delay decarbonization measures, as better technologies may be available in the future?)

It is obvious that these questions are answered very differently by the various players (companies, politicians, society).

A close collaboration between academia and industry is needed to tackle these challenges: Academia may provide the knowledge to identify, structure and frame the described challenges and identify, develop and evaluate potential technical and societal solutions. But bringing all these ideas into life, financing and upscaling the solutions can only be done with the help of motivated entrepreneurs ready to re-invent the chemical industry, acting within the limits of the planetary boundaries and defossilizing its feedstocks and energy. That's why I believe that we will need the „Journal of Business Chemistry" in the future, too. It is a relevant platform for collaboration: „Business meets chemistry" and „Academia meets practice". This is in a nutshell how we create impact for the sustainable development of the chemical and pharmaceutical industries.

Interview conducted by: Andrea Kanzler

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Research Paper

Uday Grover*, Janvee Garg and Prof. Anil Kumar Singh*****

From brass to brilliance: Frugal innovation for safer public spaces

This study explores the application of brass, noted for its cost-effective antimicrobial properties, as a frugal innovation to enhance public sanitation in high-traffic public health settings such as hospitals and public transport systems. Underpinned by the principles of frugal innovation - resource efficiency, affordability, accessibility, and sustainability, this research assesses the effectiveness and economic viability of various brass applications for microbial control on high-touch surfaces. Through an exploratory review of the literature, this study identifies that brass applications not only reduce the need for frequent sanitation but also ensure durability and long-term effectiveness in public spaces. Findings highlight that integrating brass in public infrastructure significantly lowers infection rates and healthcare costs, aligning with frugal innovation's focus on maximizing value with minimal resources. The study contributes to public health strategies by demonstrating brass's role in sustainable and economically advantageous solutions.

Introduction

In today's rapidly evolving world, marked by significant technological advancements and pressing societal demands, the quest for sustainable and cost-effective solutions to global challenges is more pressing than ever. Amid these challenges, the concept of "frugal innovation" has emerged as a pivotal approach, particularly valued in resource-limited settings (Hindocha et al., 2021; Rao, 2013; Zeschky et al., 2011). Frugal innovation, which focuses on maximizing resource efficiency while minimizing costs, is crucial for addressing public health challenges, especially in contexts facing rising healthcare costs and an increased prevalence of infectious diseases (Anderson & Lillis, 2010; Bhatti et al., 2017; Tiwari & Herstatt, 2012). Recent literature highlights the importance of such innovations in efficiently managing public health threats (Levänen et al., 2022; Miesler et al., 2020; Sarkar, 2021; Sarkar & Mateus, 2022). Specifically, brass, known for its cost-effective antimicrobial properties, offers a practical solution to enhance sanitation in public spaces - areas vulnerable to the rapid spread of infections (Borkow & Gabbay, 2005; Grass et al., 2011). This study explores the strategic use of brass as a frugal innovation to improve public health safety efficiently and sustainably, aiming to fill a critical gap identified in existing research (Prahalad & Hart, 2010).

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By leveraging the long-recognized antimicrobial properties of brass, this research proposes economically viable solutions to improve sanitization in high-traffic areas such as hospitals and public transport systems (Grass et al., 2011). Integrating insights from Prahalad & Hart (2010), this study extends the dialogue on frugal innovation, illustrating how brass not only meets but enhances the principles of resource efficiency, affordability, accessibility, and sustainability.

As global concerns about infectious diseases escalate, the relevance of frugal innovation principles in public health becomes increasingly significant (Bhatti et al., 2017). This research delves into the potential of brass to revolutionize hygiene practices, potentially setting new standards in public health measures in critical settings. This investigation is guided by two pivotal research questions:
RQ1: Which form of brass application is the most economically viable and effective for killing microbes on high-touch surfaces?
RQ2: Which specific applications of brass-based technology should be prioritized for maximum cost-effectiveness and microbicidal efficacy?
These questions seek to identify brass application methods that deliver maximum value with minimal resources and to strategically implement brass-based technology in real-world scenarios to maximize public health impact. The outcomes of this study promise to reshape future sanitization practices, making them more efficient, accessible, and sustainable. Moreover, the insights from this research will equip decision-makers across various sectors with the knowledge to deploy brass-based frugal technology effectively. This study stands at the intersection of material science, public health, and innovation studies, offering valuable insights poised to influence future sanitization practices and policies. Additionally, the multifaceted applications of brass, including in textiles, underscore its role as a powerful tool for microbial control and infection prevention, ensuring a safer and more sustainable future for all.

Exploring and prioritizing brass applications for enhanced sanitization

To address Research Question 1 (RQ1), this study conducted an exploratory review that identified various brass applications currently in use or under investigation. According to the Antimicrobial Copper Alloys Group (2010), brass coatings, decals, and sprays are among the solutions being evaluated for their effectiveness in public health settings. Each application form was analyzed for its cost-effectiveness and microbicidal efficacy, as well as its durability and capability to withstand the wear and tear commonly seen in high-traffic environments (Grass et al., 2011). This analysis is crucial for ensuring long-term effectiveness and sustainability in public spaces. This revealed that different forms of brass application vary significantly in their ability to kill microbes on high-touch surfaces. Studies have shown that brass coatings, in particular, provide rapid and effective microbicidal action, which is essential for public safety (Militky et al., 2021). This finding supports the selection of specific brass applications that maximize both economic and health benefits.

To address Research Question 1 (RQ1), this exploratory review identified various brass applications currently in use or under investigation (Antimicrobial Copper Alloys Group, 2010). The authors analyzed existing research to determine the advantages and disadvantages of each form, focusing on their cost-effectiveness and microbicidal efficacy. Additionally, the durability of each application form are accessed and its capability to withstand wear and tear in high-traffic environments, crucial for maintaining long-term effectiveness in public spaces. The effectiveness of different brass application forms in killing microbes on high-touch surfaces was evaluated through the literature. This approach helped to identify which forms provide the most rapid and effective microbicidal action for ensuring public safety.

Addressing Research Question 2 (RQ2), the analysis considered the cost-effectiveness and microbicidal efficacy of these applications to identify specific areas such as doorknobs, handrails, or seating that offer the highest return on investment in terms of public health and safety. This prioritization is based on a thorough review of existing data and industry best practices.

The investigation into brass application forms has unearthed valuable insights, providing a nuanced perspective on the potential of brass-based technology to enhance sanitization practices. Significant differences in the applications and properties of red brass and yellow brass were discovered. Red brass, known for its durability and corrosion resistance, and yellow brass, favored for its malleability and aesthetic appeal, both offer unique benefits for different settings (Roche Industry, 2021). The higher copper concentration in

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red brass enhances its antimicrobial effectiveness, making it particularly valuable in healthcare settings where reducing microbial contamination is crucial (Abraham et al., 2021).

Moreover, the application of copper in textiles presents a powerful tool for microbial control. Copper-infused textiles have broad-spectrum antimicrobial properties that effectively combat various microorganisms, including antibiotic-resistant strains like Methicillin-Resistant Staphylococcus aureus (MRSA) and Vancomycin-Resistant Enterococci (VRE) (Borkow & Gabbay, 2005). These textiles not only reduce the risk of skin and wound infections but also benefit individuals with allergies or diabetes, offering a comprehensive approach to infection prevention and control in healthcare settings (Borkow and Gabbay, 2004).

In addressing RQ2, the analysis highlights the importance of prioritizing brass applications in public spaces. By strategically deploying brass-based technology in hospitals and public transportation systems, decision-makers can significantly reduce microbial burdens and the risk of disease transmission. The prioritization of high-touch surfaces ensures that brass applications are used where they are most needed, maximizing public health benefits and safety.

Assessing risks and navigating challenges in brass implementation

Despite the considerable benefits brass applications offer in bolstering public health, several risks and challenges necessitate comprehensive examination and strategic mitigation. Foremost among these concerns is the potential emergence of microbial resistance over time as a consequence of sustained exposure to brass surfaces (Michels et al., 2008; Murray et al., 2022). To address this risk effectively, continuous surveillance of microbial populations and resistance patterns is imperative to gauge the efficacy and sustainability of brass-based interventions (Grass et al., 2011; Infectious Diseases Society of America (IDSA), 2011). Additionally, stringent protocols for surface cleaning and disinfection may be warranted to prevent the proliferation of resistant strains. Environmental implications represent another critical consideration in the deployment of brass technologies, particularly concerning the disposal and potential accumulation of brass materials in ecosystems (Michels et al., 2008; Sterling Group, 2018). Conducting thorough lifecycle assessments and implementing sustainable disposal practices are essential to minimize the environmental footprint of brass interventions (Johansson et al., 2020). Exploring alternative materials or surface treatments with lower environmental impacts could provide viable solutions to mitigate these concerns while maintaining efficacy. Financial barriers, particularly in economically disadvantaged settings, significantly hinder the widespread adoption of brass technologies. Addressing this challenge necessitates innovative financing mechanisms and partnerships with governmental and non-governmental organizations to offset initial investment burdens and facilitate broader implementation (Cioffi & Rai, 2012). The durability and maintenance requirements of brass surfaces also demand attention. Variations in application methods and environmental conditions can influence the longevity and effectiveness of brass interventions, necessitating tailored maintenance protocols to ensure sustained antimicrobial efficacy and operational efficiency (Mehtar et al., 2008). Equitable distribution and access to brass-based interventions are fundamental considerations to prevent exacerbating health inequalities. Proactive measures to address disparities in healthcare infrastructure and resource allocation are imperative to ensure that vulnerable populations benefit equitably from brass technologies (Spellberg & Gilbert, 2014). Lastly, successful integration of brass into existing public health infrastructure requires collaboration and coordination among diverse stakeholders. Establishing clear communication channels, standardizing implementation protocols, and addressing regulatory requirements are essential for seamless deployment and sustained effectiveness (Weber et al., 2010).

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Frugal innovation and brass-based sanitization

Frugal innovation, a strategy increasingly recognized for its potential to address complex challenges with minimal resources, emphasizes creating solutions that are simple, affordable, accessible, and sustainable. This approach aligns with the pressing need to develop sanitation solutions that are not only effective but also economically and environmentally viable, especially in high-traffic public areas (Hindocha et al., 2021). These principles are particularly relevant given the global context of resource scarcity, heightened market demand for sanitation, rapid technological advancements, and significant societal needs (Basu et al., 2013; Soni & T. Krishnan, 2014).

The core objective of this research is to identify the most straightforward and effective applications of brass for enhancing sanitization. By investigating various forms of brass applications, the study aims to determine which methods can be seamlessly integrated into existing public health infrastructures without causing significant disruptions or necessitating extensive maintenance routines (Antimicrobial Copper Alloys Group, 2010). This focus on simplicity ensures that the proposed solutions are not only user-friendly but also conducive to rapid deployment in diverse settings. This exploration is critical as it aligns with the frugal innovation's emphasis on simplicity, which not only facilitates ease of use but also promotes rapid adoption in varied public health contexts (Dabić et al., 2022; Khan & Melkas, 2020).

Affordability remains a cornerstone of frugal innovation.

The study compares the costs associated with various brass application forms, highlighting those that provide the best value for money. This emphasis on cost-effectiveness is crucial, particularly in sectors like healthcare and transportation where budget constraints are common (Bhatti et al., 2017). By demonstrating the economic benefits of brass applications, this research supports broader adoption and implementation across financially diverse settings (Abraham et al., 2021). This study highlights the cost benefits associated with various brass applications, identifying those that offer the most significant economic advantage.

Enhancing accessibility and sustainability

Accessibility is a dual concern: Ensuring that all users can benefit from improved public health measures and that these measures are easily implemented across various infrastructures. The study also assesses the durability of different brass forms, providing insights into which are most likely to endure in high-traffic environments, thus enhancing their sustainability. The antimicrobial properties of brass contribute to this sustainability, offering long-lasting effectiveness that helps prevent frequent replacements or upgrades (Borkow & Gabbay, 2005; Dauvergne & Mullié, 2021; Vincent et al., 2016). The research examines how brass applications can be made accessible across different public infrastructures and sustainable over time. Durability tests of various brass forms are evaluated to ensure long-term effectiveness, particularly in environments with high public interaction, supporting ongoing efforts to reduce environmental impact (Yu et al., 2020).

Addressing market and societal needs

The research directly responds to a clear market demand for more robust sanitization measures, a need intensified by the ongoing challenges posed by infectious diseases. Brass, with its proven antimicrobial properties, is positioned as a viable solution to enhance sanitization in public spaces, which are critical nodes in the spread of diseases. This study not only explores the efficacy of brass applications but also how these can be optimized to meet the pressing societal need for improved public health safety. By responding to the urgent demand for enhanced sanitization practices, this study positions brass as an essential tool in public health strategy, especially crucial in mitigating the spread of infectious diseases in high-traffic environments (Vardoulakis et al., 2022). It emphasizes the role of technological innovations in adapting these solutions to meet societal expectations and market demands effectively.

Extending antimicrobial applications beyond healthcare

The effectiveness of copper, and by extension brass, extends beyond healthcare environments into places such as retirement homes, kindergartens, and offices. Inkinen et al., (2017) conducted a study replacing conventional materials with copper in these settings on high-contact surfaces like door handles, light switches, and toilet flush buttons. Their findings indicated that these copper surfaces maintained significantly lower bacterial loads than those made with standard materials, proving copper's effectiveness

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across a variety of settings. Such empirical evidence supports broader implementation of brass to ensure public safety and health across different environments, leveraging its inherent antimicrobial properties.

Mapping the frugal innovation principles with brass applications

In this study, the authors have explored how the principles of frugal innovation, specifically designed to leverage minimal resources for maximum benefit, are effectively applied through the use of brass in public health initiatives. Below, the authors detail the key drivers of frugal innovation and map these directly to the characteristics and benefits of brass applications.

Resource Efficiency

Central to frugal innovation is the optimization of resource use to achieve more with less (Dabić et al., 2022). Brass, known for its durability and antimicrobial properties, exemplifies this principle. Its composition, particularly the copper content, provides prolonged antimicrobial activity, which is crucial in high-traffic public health environments. This characteristic significantly reduces the need for frequent replacements and maintenance, offering a sustainable solution that aligns with the frugal innovation's emphasis on resource efficiency.

Cost-Effectiveness

Frugal innovations aim to deliver financial sustainability by minimizing cost without compromising quality (Sarkar & Mateus, 2022). The implementation of brass as an antimicrobial surface in public health settings, while initially more costly, is offset by the reduction in healthcare-associated infections (HAIs) and subsequent savings on treatment and sanitation costs. Studies have shown that environments utilizing copper-alloy surfaces, like brass, experience a measurable decrease in infection rates, which directly translates to cost savings (Dauvergne & Mullié, 2021).

Accessibility

Ensuring that innovations are readily accessible to a broad audience is another cornerstone of frugal innovation (Albert, 2019; Tiwari & Herstatt, 2012). Brass applications in public spaces, such as hospitals and transport systems, make antimicrobial protection accessible to all users, contributing to widespread public health benefits. The ease of integrating brass into existing infrastructures replacing common touch surfaces like door handles and railings enhances its accessibility and practicality.

Sustainability

The long-term viability of an innovation is essential in frugal innovation (Albert, 2019). Brass not only offers immediate antimicrobial effects but also remains effective over time, even with repeated exposure to pathogens. This enduring effectiveness ensures that brass surfaces do not require frequent chemical cleanings or replacements, supporting environmental sustainability and ongoing public health safety (Grass et al., 2011). To visually synthesize how these principles of frugal innovation are applied through brass in public health, the following table 1 categorizes each principle alongside corresponding attributes of brass:

Table 1: Mapping the frugal innovation principles and application of Brass

Frugal Innovation Principle	Application in Brass Use	Impact on Public Health
Resource Efficiency (Dabić et al., 2022)	Durable, long-lasting antimicrobial action	Reduces need for frequent maintenance
Cost-Effectiveness (Sarkar & Mateus, 2022)	Reduces HAIs, lowers healthcare costs	Financial savings over long term
Accessibility (Albert, 2019; Tiwari & Herstatt, 2012)	Easy to integrate into existing structures	Widespread public health benefits
Sustainability (Albert, 2019)	Endures without frequent replacements	Minimizes environmental impact

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Concluding discussion and implications

This research has delved into the potential of brass applications to enhance sanitization in public health settings through the principles of frugal innovation, primarily focusing on their economic viability, sustainability, and accessibility. The investigation has confirmed that brass, provides a cost-effective solution for reducing the microbial presence on frequently touched surfaces. This aligns with findings by Borkow & Gabbay (2005) who noted the significant antimicrobial properties of copper alloys, enhancing their utility in public health applications. However, while brass offers long-term savings due to reduced disease transmission and decreased need for replacements, the initial costs can be prohibitive, particularly in under-resourced settings. The economic challenge posed by the higher initial cost of implementing brass applications highlights a significant barrier.

Despite these economic concerns, the study highlights the importance of accessibility in public health innovations. Simple and scalable solutions such as brass applications can significantly improve hygiene across diverse settings, particularly in areas lacking advanced medical infrastructure (Vincent et al., 2016). This approach not only aligns with global health priorities aimed at reducing the spread of infectious diseases but also embodies the frugal innovation mandate to create sustainable and accessible solutions (Bhatti et al., 2017).

However, the adoption of new technologies must be managed carefully to avoid potential downsides, such as increased microbial resistance or adverse impacts on existing environmental management systems (Yu et al., 2020). These considerations point to the need for a balanced approach in the implementation of brass-based technologies, ensuring that while they meet the immediate needs of public health safety, they do not inadvertently create new challenges.

The intersection of material science, public health, and innovation studies in this research highlights a multidisciplinary approach to addressing significant challenges in healthcare environments. At its core, this study leverages material science to explore the properties and applications of brass, specifically its antimicrobial effectiveness due to its copper content. Material science not only provides the technical basis for understanding how brass combats pathogens on surfaces but also guides the development of various brass applications that are tested for durability and efficacy. By examining the alloy's composition and interaction with microbial agents, material science contributes to creating solutions that are both innovative and practically applicable in high-traffic public areas. The implications of using brass are directly linked to public health outcomes. This study examines how the integration of brass in public settings such as hospitals and public transportation can reduce the spread of infections, thereby enhancing public health safety. The effectiveness of brass in lowering infection rates and potentially decreasing the incidence of healthcare-associated infections (HAIs) aligns with the goals of public health to safeguard communities and improve environmental health conditions. The research here responds to urgent public health needs by providing a preventive strategy against microbial transmission, which is a pressing concern in public health management. Innovation studies provide the framework for applying frugal innovation principles to the use of brass in public health settings. This field explores how innovative, cost-effective, and accessible solutions can be developed and implemented to meet specific needs, particularly in resource-constrained environments. The study's focus on frugal innovation through the use of brass underscores the importance of developing practical, scalable, and economically viable technologies that can be widely adopted. It addresses how innovation in material applications can be a game-changer in public health strategies, especially in enhancing the sustainability and accessibility of health interventions. The convergence of these three domains in the study leads to a comprehensive understanding of how advanced materials can be utilized to meet public health needs while adhering to the principles of innovation. By integrating material science with public health imperatives and innovative application strategies, the research not only contributes to the academic discourse but also provides actionable insights for policymakers, healthcare providers, and other stakeholders in the health sector. This multidisciplinary approach ensures that the solutions developed are not only scientifically sound and effective but also aligned with the broader objectives of public health enhancement and sustainable innovation.

While brass is extensively discussed in this paper for its antimicrobial properties and potential applications, it's essential to consider a range of alternative materials to provide a comprehensive understanding of available

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options. In addition to brass and copper, materials such as titanium dioxide (TiO_2), silver, and nanotechnology-based solutions offer unique advantages and applications in enhancing public sanitation. Titanium dioxide is a versatile compound known for its photocatalytic properties, making it effective in degrading organic pollutants and inhibiting microbial growth under UV light exposure (Armaković et al., 2022). TiO_2-based coatings have shown promise in reducing the survival and proliferation of various pathogens, including bacteria, viruses, and fungi, on surfaces such as medical equipment, countertops, and packaging materials and it continuously generate reactive oxygen species upon exposure to light, disrupting microbial cell membranes and DNA and providing long-lasting antimicrobial activity (Kumaravel et al., 2021). TiO_2 coatings are compatible with a wide range of substrates, transparent, and environmentally friendly, making them suitable for diverse applications in public health settings (Tian et al., 2023). Silver has long been recognized for its antimicrobial properties and has been widely used in healthcare settings to inhibit microbial growth on surfaces and medical devices (Lansdown, 2006). Silver-based coatings or nanoparticles have shown efficacy in reducing the survival of bacteria, viruses, and fungi, making them suitable for various applications, including wound dressings, catheters, and water purification systems (Xu et al., 2020). While silver offers effective antimicrobial protection, concerns have been raised regarding potential toxicity and environmental impact associated with its widespread use, necessitating careful consideration of these factors in decision-making (Bruna et al., 2021). Advancements in nanotechnology have led to the development of novel antimicrobial materials with enhanced efficacy and versatility. Nanoparticles, such as silver nanoparticles, zinc oxide nanoparticles, and graphene oxide, exhibit strong antimicrobial properties due to their high surface area-to-volume ratio and unique physicochemical properties and these nanoparticles can be incorporated into coatings, textiles, and medical devices to provide durable and effective antimicrobial protection (Sirelkhatim et al., 2015). However, challenges remain in scaling up production, ensuring safety, and addressing potential environmental concerns associated with nanomaterials (Ray et al., 2009). While brass remains a promising option for enhancing public sanitation, exploring alternative materials such as titanium dioxide, silver, and nanotechnology-based solutions can offer additional options for addressing microbial contamination in public spaces. Each material presents unique advantages and considerations, highlighting the importance of evaluating their suitability based on specific application requirements and environmental considerations.

Limitations and scope for future research

Despite the promising findings, this study is subject to several limitations that should be considered when interpreting the results. The study primarily draws on existing research and industry best practices, which may not be universally applicable. The economic assessments of brass applications were primarily based on theoretical models and retrospective analyses, which may not fully capture the real-world complexities of implementing such technologies in diverse settings. Furthermore, the study's focus on brass might limit the exploration of other potentially more cost-effective or sustainable materials. Additionally, the resistance development among pathogens due to continuous exposure to brass surfaces has not been fully explored, which could undermine the long-term effectiveness of these interventions. Given the identified limitations, future research should focus on several areas to expand the understanding and application of brass-based technologies in public health. Prospective studies are needed to evaluate the real-world efficacy and cost-effectiveness of brass installations in various environmental conditions and usage patterns. Such studies could help validate the findings from this research and adjust implementation strategies based on empirical data. Additionally, comparative studies involving other antimicrobial materials could offer insights into the relative performance and sustainability of different options, guiding resource allocation in public health investments. Research into the potential resistance development among pathogens in response to continuous exposure to brass surfaces is also crucial. Understanding these dynamics will inform the design of interventions that minimize the risk of creating resistant microbial populations. Lastly, interdisciplinary research combining material science, public health, and behavioral sciences could explore how the design and deployment of antimicrobial technologies influence user behavior and overall public health outcomes. Such research would provide a holistic view of how innovative materials can be effectively integrated into public health strategies to maximize their benefits and sustainability.

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Interview

with Dr. Steffen Kanzler*

A conversation about artificial intelligence at Evonik

What are current topics and trends in the chemical industry?

Thanks for having me. So far 2024 has been another challenging year. We saw a lot of supply chain disruptions and several players were facing production issues. Additionally, competition in Europe was highly active and many Asian players seem to have taken an interest in the European market. Volatility of energy costs and changing regulations and policies led many chemical companies to reevaluate their assets and production plant setups.

From our customers perspective, sustainability and circular economy principles have gained importance. We recently conducted a survey among our customers, and it clearly showed that sustainability will be a key topic for this year and going forward. Providing information on product carbon footprints, life cycle analysis or bio-based content in our products has become an opportunity to differentiate yourself from competition. Many customers have sustainability scorecards for their suppliers and manage their business to a certain degree according to their sustainability scores. Evonik is a pioneer in this area. We aspire to create sustainable, value-added solutions for our customers. Evonik has integrated sustainability into the corporate strategy, from research & development through portfolio management to corporate culture. Our goal is to increase the share of our portfolio with strong positive sustainability profiles to over 50% by 2030, today we are at about 43%. Evonik has also committed to support the objectives of the Paris Agreement on Climate Change. For instance, Evonik commits to the Science Based Targets initiative (SBTi) and aims to reduce our scope 1 and 2 emissions by 25 percent, while scope 3 emissions are targeted to be reduced by -11%. All this is in line with the SBTi target level of “well below 2°C”. Another key topic for 2024, and probably for the coming years, is digitalization and artificial intelligence. I see a lot of activity in this area by many chemical companies. Data has become important across all our businesses; it is almost like a new feedstock for us. Here as well Evonik is an early adaptor, digitalization and AI are key elements of our strategy and Evonik has been actively looking at AI and its application within the chemical industry for many years now.

How do you see artificial intelligence impacting the chemical industry in the next 5-10 years?

We see artificial intelligence having a significant impact on our industry in the next 5-10 years. There is potential for benefits of AI in the automation of standard manual tasks in customer service and supply chain, such as order intake, no touch orders, forecasting, or production planning optimization. AI can definitely help here; however, I see it rather being a tool that complements humans or frees up their time for other tasks such as direct customer communication. AI is usually good when there is a lot of data and high quality in the data,

* Marketing Director at Evonik

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with limited bias. For this application usually prerequisites for a successful implementation of AI are met.

In addition to these areas, we see a use case for AI for innovation in the chemical industry. For instance, AI can be used to screen for new molecules and predict their properties, which saves us time and cost for testing, and it may allow us to speed up the development of new products and bring them to market faster. There are large databases of molecule properties available with which one could train AI and then predict the behavior of new molecules, e.g. for finding new hardeners for coatings that deliver great heat resistance or chemical resistance properties. I have seen already some academic publications in this area where AI accurately predicted molecule properties, in the future this could be a game changer for the chemical industry, innovation is key for any specialty chemical company, and it is cost and time intensive. Thus, any help of AI in this area is highly welcome.

Other areas where we see potential for AI in the chemical industry include process optimization, quality control, and predictive maintenance. By using AI to analyze data from sensors and other sources, we can identify potential issues in production before they occur and take corrective action to prevent downtime and improve product quality. Predictive maintenance is a keyword here and for accident prevention I can see that AI could be very useful in the future. AI could be trained with various data from production plants sensors on "close calls, or prevented incidents" as well as actual production accidents and plant failures and then this AI could be used to predict future cases and help to prevent those.

Overall, I believe that the use of AI in the chemical industry will continue to grow, and we will see more applications emerge in the coming years. This technology has the potential to transform our industry and help us stay competitive in an increasingly complex and challenging market.

Before we continue in to detail with AI; many of our readers are currently studying business chemistry and you are a business chemist working currently in an interdisciplinary position, tell us a bit about your career?

I joined Evonik in 2012 after completing my PhD and I took over a project manager role, which was similar to an inhouse consulting role. After about two years in that role, I joined the business line Crosslinkers and more specific their new business development group, where I was responsible for composite applications of our amine hardeners. Then, I had the opportunity to move to the USA as a business development manager for North America and sales rep for Mexico. During my time in the US, Evonik offered me a marketing position, and from 2017 on I was in charge of marketing for the market segments Adhesives and Composites. At the end of 2020 after about 4.5 years in the US, I moved back to Germany and joined the business line High Performance Polymers, here I held a marketing position for our Vestakeep® products, with a focus on automotive and aerospace applications. After two years in this role, I was offered a marketing director position back at the business line Crosslinkers, which I happily accepted. Here I am responsible for our Coatings business in EMEA. Furthermore, we are working on a lot of projects regarding digitalization. Evonik is also looking into different trending topics, including future applications of AI in the chemical industry.

Can you provide an example of how your company is currently using AI to improve efficiency or productivity in the chemical manufacturing process?

Yes, there are a couple of projects and applications that I can name here. Actually, Evonik sees itself as a pioneer for digitalization and the application of AI in the chemical industry. For instance, we are the first chemical company to participate at the MIT-IBM Watson AI Lab based on the MIT campus in Cambridge, Massachusetts. Experts from academia and industry are working together to better understand AI and its application potential for the chemical industry among other topics. Here research is done on AI supported material discovery, formulation technology, knowledge management, market analysis and more in general on decision making, e.g. how AI can help to make better and faster decisions. We have an active partnership with IBM on topics like this since 2017 and we have completed several projects, i.e. our scientists no longer have to search for expert knowledge like for a needle in a haystack. Instead, decades of knowledge and information are now easy to search and to analyze intuitively with support of AI, our chemists can easily explore and compare formulations and their related properties to come up with new developments and innovative products.

One of our AI applications is COATINO®, our virtual formulation assistant, which is available free of charge to the entire paint & coatings industry. Coatings and paint formulators can go on our webpage www.coatino.com and can request AI-based additive recommendations for their specific applications, for example with individual guiding formulations for pigment concentrates. The AI application COATINO® now can even be used via voice control. The recommendations by COATINO® and its algorithms rely on both AI-based technology and machine learning principles. Evonik operates a high-throughput equipment that tests and evaluates up to 120 coating formulations per day and feeds these results into the continuous improvement of COATINO®. Besides large amounts of data the AI tool is of course also enriched by years and years of experience of Evonik's additive experts. When using COATINO® formulators can select from over 200 product properties and effects to obtain tailor-made and weighted recommendations. In theory 1070 property combinations are possible, and the tool includes around 1,900 existing and tested guiding formulations. Additionally, COATINO® can calculate individual formulations for all types of pigment concentrates and the data pool it is basing the recommendations on is constantly growing. Many of our clients really appreciate the voice command option, because, if unexpected challenges arise in the laboratory, technicians and scientists can obtain technical information on additives and still have both hands free to continue their work in parallel.

A decisive factor in the development of COATINO® was the creation of maximum transparency for the customer. The recommended products can be dynamically compared with each other, so that the customer can grasp the differences in a few seconds and thus make their decision. A total of almost 300 products are available to choose from, including defoamers, dispersing additives, and matting agents. COATINO® sends out all technical, regulatory, and safety data sheets conveniently via the watch list if required.

Another application of AI at Evonik is the SciTai which stands for Scientific Technical Support by AI, one of first projects that was initiated as part of the strategic partnership with IBM. This AI tool helps Evonik compound experts to get easier access to the accumulated knowledge of internal research results via an intelligent graph database, consisting of over one million nodes connected with over 14 million links. The result of this lighthouse project is a knowledge platform with logically linked information from various sources, that represent over 20 years of research, digitally available in one central place. SciTai also has the capability to predict material properties and can give formulation recommendations based on AI.

Finally, I want to mention our self-learning Market Intelligence Platform CRISP (Cognitive Raw Materials Intelligence Service Platform) at Evonik Procurement. The idea for this AI application emerged in 2016, when it became more and more clear that the growing quantity of digital information on raw material prices, different indices, market volatilities and emerging and disappearing players made evaluation by humans very time consuming and difficult. Instead of having sourcing managers do the market research themselves e.g. going on a hunt for information, the idea was that the relevant information should come to them with the help of AI. For that the AI searches news sites from around the world, social media and market reports, after that CRISP autonomously selects the relevant information and then provides the information to the user in form of a personalized newsfeed, these reports will then be evaluated by our sourcing managers of which the AI then learns for future reports. In multiple cases our users of CRISP report that the AI recommended them information that turned out as highly relevant, which they would not have found without the AI, e.g. in one case CRISP recommended an article from a foreign newspaper that mentioned an event which was a key piece of information in refining a sourcing strategy for a certain raw material. In sourcing speed is of the essence and early warning signs on supply disruptions due to incidents at suppliers or transportation route disruptions often are first discussed on social media before they are picked up by traditional news channels. CRISP picks those up and helps our sourcing managers to get a head start in reacting to sudden changes.

How do you ensure the accuracy and reliability of AI-generated data in your operations?

Evonik ensures the accuracy and reliability of AI-generated data in our operations by following a rigorous process. First, we carefully select and curate high-quality data that is relevant to the specific task at hand. We then use validation techniques such as comparing the AI-generated data to original true data or using statistical methods to ensure that the data is accurate and reliable. Once the AI model is deployed, we monitor its performance using automated monitoring systems and regularly review its output to ensure that it continues to generate accurate and reliable results. We also continuously improve the AI model by retraining it on new data and fine-tuning its parameters to ensure that it remains accurate and reliable with time. In addition, we

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have a team of experts who are responsible for overseeing the AI-generated data and ensuring that it meets our high standards for accuracy and reliability. This team works closely with our data scientists and engineers to ensure that the AI-generated data is used effectively in our operations and that any issues are quickly identified and addressed.

What challenges have you faced in implementing AI technology in the chemical industry, and how have you addressed them?

We have faced several challenges in implementing AI technology. One major challenge is the data quality and availability. We have a lot of data, but it is often scattered across different systems, and the quality of the data may not be sufficient for training AI models in some cases. To address this, we have invested in systems and processes to ensure that data is properly collected, stored, and maintained. We have also explored partnerships with data providers and other companies to access additional data sources, and of course we collaborate with AI experts, like the MIT-IBM Watson AI Lab, which I mentioned earlier.

Another major challenge are regulatory concerns. The chemical industry is heavily regulated, and there may be concerns about how AI technology will impact compliance with regulations. To address this, we have worked closely with regulatory bodies to ensure that our AI systems comply with all relevant regulations and guidelines, and we continuously work here to be compliant.

Additionally, Evonik has invested in personnel that has the necessary knowledge for employing AI in the chemical industry. Evonik has hired data scientists, engineers, and other AI experts and we have also partnered with AI service providers and other companies to access specialized expertise, for instance regarding chatbot technologies.

Finally, the implementation of AI technologies required significant changes to existing processes and workflows, which sometimes can lead to skepticism from employees or customers. To address this, we have invested in change management processes and communicated the benefits of AI technology to employees and customers, and we are providing a lot of training opportunities. We have also involved employees in the implementation process to ensure that their concerns and feedback are addressed.

Overall, we recognized early that implementing AI technology in the chemical industry requires significant investment and effort. However, we believe that the benefits of AI technology, including improved efficiency and safety, and potentially also for sustainability, make it a worthwhile investment for our company and the industry as a whole.

How do you balance the potential benefits with the risks of AI in the chemical industry?

At Evonik we of course also recognize the risks associated with AI. One of the most significant risks of AI is „garbage in, garbage out“. This occurs when the quality of the data used to train the AI model is poor, resulting in inaccurate predictions and maybe wrong decisions. Therefore, data quality is always one of our main criteria when we start to train an AI model for a project. AI algorithms rely heavily on large data set, but also on high quality data, and if the data is incomplete, inconsistent, or inaccurate, it can lead to incorrect problems that one might notice only after a while. We always try to have processes in place to identify and correct any data quality issues, which sometimes is difficult because what the AI actually does is often kind of a black box. Thus, we work with experts to get transparency on the inner workings of our AI algorithms.

Bias is another significant risk associated with AI. AI algorithms can be biased if they are trained on data that is biased, or if the algorithm itself has inherent biases. We work hard to ensure that the data used to train the AI model is free of biases. Everybody in the AI field knows about the case at Amazon in 2018, when they shut down their AI recruiting tool, after realizing that it was discriminating against women. Incidents like that, we try to avoid from the start of course. Additionally, we regularly monitor and audit our AI systems to identify and correct any biases that might occur.

Overall, in balancing the potential benefits with the risks of AI in the chemical industry, we always prioritize safety and quality. Evonik ensures that any AI system that gets implemented is thoroughly tested and validated by our experts before it is used. I am looking forward to many additional applications and use cases of AI within Evonik, for the chemical industry the benefits can be huge and I feel we are still in the early phases of the adaption of this new technology and there is much more to come.

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Commentary

Dr. Andreas Konrad*

How artificial intelligence can be used in the chemical industry

Introduction

The chemical industry is discovering more and more opportunities to leverage the power of artificial intelligence (AI). Although AI as an active scientific discipline is around since the 1950s (Wooldridge, 2018) and has gone through several waves, it now seems to be on the radar of almost every chemical company. While the integration of AI in chemical engineering is not novel, its comprehensive application and potential are yet to be fully realized (Venkatasubramanian, 2019). Energy and oil price volatility as well as supply and demand fluctuation force the chemical industry to be more agile in order to adapt faster to this new market environment. Additionally, stakeholders on all sides expect significant efforts regarding environmental responsibility, sustainability and circularity. Furthermore, innovation is a key driver of competitive advantage and differentiation in the chemical industry, however with more stringent regulations and pressure on innovation budgets, identifying and then speeding up the most promising R&D projects is more important than ever. Hence, AI is a critical tool in the transformation the chemical industry is facing.

According to a recent survey conducted by IBM (Womack et al., 2020), an 80% of managers within the chemical industry acknowledge the imminent transformative influence of artificial intelligence on their business operations within the next three years. This statistic underscores the industry's recognition of AI as a pivotal driver of change, signaling a paradigm shift in how chemical companies operate and innovate. The survey further describes major areas where AI is anticipated to make significant inroads, with research and development leading at 74%, followed by production optimization at 61%. Additionally, AI is expected to play a pivotal role in forecasting and planning, with 47% of respondents identifying it as a critical area for AI implementation. Moreover, risk management emerges as another focal point for AI integration, with 58% of surveyed managers recognizing its potential to enhance decision-making processes and mitigate operational risks (Womack et al., 2020). To summarize recent activities this commentary will explore key areas for AI application within the chemical industry.

AI applications in the chemical industry

Ensuring safety remains paramount in chemical manufacturing, where the repercussions of accidents can be catastrophic. AI offers a transformative solution by leveraging predictive analytics to anticipate potential hazards and preemptively mitigate risks. Machine learning algorithms, particularly supervised learning models, are well-suited for this task. For instance, AI systems can analyze historical data to identify patterns indicative of impending accidents, enabling proactive intervention (Mao et al., 2019). Similar to the use of AI, for instance in the radiology space, where the AI was trained with images of abnormalities from diagnostic scans and can now help to improve diagnostic accuracy and also reduce the radiologists workload (Giansanti et al., 2021; Kelly et al., 2022; Mun et al., 2020), AI in the chemical industry could be trained with critical production plant data before accidents had happened in the past, to better predict failures in the future. Furthermore, AI can revolutionize safety training by providing immersive virtual reality experiences that simulate hazardous scenarios. Today AI-driven simulations can facilitate virtual testing of safety protocols and emergency response strategies, and augmented reality is used to prepare the workforce and helps minimizing the likelihood of incidents (Chiang et al., 2022). By continuously adapting to evolving safety standards and regulations, AI-driven training

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modules ensure that employees in the chemical industry are up to date with best practices and protocols.

As the IBM survey demonstrates, AI has found its way into R&D and innovation departments. AI's capacity to analyze vast datasets unlocks unprecedented avenues for innovation in molecule design. Through machine learning algorithms, researchers can expedite the discovery of eco-friendly materials and chemicals, thereby avoiding the reliance on conventional, environmentally harmful substances (Schmidt et al., 2017). For instance, AI-driven simulations enable virtual screening of molecular structures, identifying compounds with desirable properties for various applications. This approach not only accelerates the development of new products but can also minimize the environmental footprint associated with traditional synthesis methods. Deep learning algorithms, particularly generative models, hold promise for material design tasks. For example, generative adversarial networks (GANs) can generate novel molecular structures with desired properties by learning from existing chemical data. Real-life applications include the use of GANs to design organic photovoltaic materials with improved efficiency and stability, accelerating the development of renewable energy technologies. By leveraging machine learning algorithms, researchers can expedite the discovery of novel catalysts and reaction pathways, thereby enabling also the development of greener synthesis methods (Doan et al., 2020). Through AI-driven simulations, scientists can better predict molecular interactions, revolutionizing the way new materials and compounds are designed and synthesized. Furthermore, AI-driven synthesis holds promise for decentralized manufacturing and on-demand production, offering a pathway to reducing reliance on centralized facilities and transportation networks. By integrating AI into small-scale reactors and production units, chemical manufacturers can customize processes to meet localized demand while minimizing environmental impact.

Additionally, AI is driving innovation in the field of green chemistry, where the emphasis is on designing processes that minimize or eliminate the use and generation of hazardous substances. Through AI-enabled predictive modeling, researchers can identify reaction conditions and solvent systems that maximize yield while minimizing waste and energy consumption. For example, AI algorithms can analyze reaction databases to identify sustainable alternatives to traditional solvents and reagents, leading to more efficient and environmentally friendly synthesis routes. Moreover, AI is facilitating the development of autonomous chemical synthesis platforms, where robotic systems can perform complex synthesis tasks with minimal human intervention. These platforms leverage AI algorithms to plan and execute synthesis routes, monitor reaction progress in real-time. However, those applications are still rather in the future. According to Walter Grüner, Head of IT & Digitalization at Covestro: "[…] the chemical industry is predestined for the use of AI because we have a lot of complex processes going on that cannot be described by fixed rules. They are not suitable for automation. We rather need learning systems to which we grant a certain degree of decision-making autonomy. In doing so, we focus primarily on the development of systems that work in a complementary manner to humans and support their abilities." (Rothbarth & Weiße, 2023).

However, when AI complements chemical engineers very often process optimization are the result. By harnessing AI-driven predictive modeling with human supervision chemical plants can dynamically adjust process parameters in real-time, optimize energy consumption and resource utilization (Shinkevich et al., 2021). Moreover, AI-enabled process monitoring facilitates early detection of inefficiencies, allowing for timely intervention and continuous improvements. Machine learning techniques, such as reinforcement learning, are particularly well-suited for process optimization tasks. For example, AI systems can learn optimal process control strategies by accessing historical data complemented by input from experienced plant engineers. Through iterative learning, these systems then can adapt and refine control protocols to maximize energy efficiency and minimize waste generation. Real-life examples include the use of reinforcement learning algorithms to optimize reactor operations in chemical plants, leading to significant reductions in energy consumption and production costs (Shinkevich et al., 2021).

For example in 2021 in Japan 20 chemical companies started to collaborate on the development of an AI based system to shorten development times on new durable and heat-resistant materials. The companies share their data and also extract training data from patent databases. In doing so they expect to reduce development times from decades down to several months (Goto, 2020). The AI powered approach again complements traditional development

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methods which relied on researchers‘ experience along with educated guesses or trial and error.

Another area were AI will play an important role for the chemical industry is supply chain optimization.
Efficient supply chain management is instrumental in minimizing the waste of resources in the highly complex chemical industry. AI-driven analytics offer support by optimizing inventory management, transportation logistics, and demand forecasting. By analyzing historical data and market trends, AI systems can predict demand fluctuations with high accuracy, enabling proactive inventory replenishment and minimizing stockouts (Chiang et al., 2022). Predictive analytics techniques, such as time series forecasting and anomaly detection, are well-suited for supply chain optimization tasks. For example, AI systems can analyze historical sales data to forecast future demand patterns and optimize inventory levels accordingly. Additionally, anomaly detection algorithms can identify deviations from expected supply chain behavior, allowing for proactive risk mitigation and contingency planning. Real-life examples include the use of predictive analytics to optimize inventory management in chemical supply chains, reducing carrying costs and improving overall efficiency. Furthermore, AI-powered routing algorithms optimize transportation routes, reducing fuel consumption and emissions associated with product distribution and AI can help by including weather data with operational data to adjust routing, and lead times (Womack et al., 2020).

Some 81% of companies surveyed by IBM, which they call AI champions also started to include AI to improve the customer experience. For instance Evonik has launched COATINO a virtual assistant that can help coating and paint formulators with recommendations on which coating additives to use or what pigment concentrations are best for a specific customer application (Womack et al., 2020). Other companies started to use AI in the customer service department, e.g. by automating order intake via AI, with the goal to achieve zero-touch orders, i.e. human actions required to complete an order from order-in-take until invoicing are reduced to near zero. This frees up resources for more value generating tasks.

Conclusion

In conclusion, AI will be a powerful tool for the chemical industry. However, AI also comes with risks. While the integration of AI holds immense promise for driving sustainability within the chemical industry, several challenges must be addressed to realize its full potential. Firstly, the development of AI-driven solutions requires interdisciplinary collaboration between industry stakeholders, academia, and government agencies. This collaboration is essential for leveraging diverse expertise and resources to tackle the complexities of the chemical industry. Secondly, concerns regarding data privacy, security, and ethical considerations will require robust regulatory frameworks to ensure responsible AI deployment (Venkatasubramanian, 2019). As AI technologies become more pervasive in chemical manufacturing, it is essential to establish clear guidelines and standards for data collection, sharing, and usage to protect intellectual property and ensure compliance with regulatory requirements. Moreover, continued investments in research and development are imperative to enhance AI capabilities and tailor them to the unique needs of the chemical industry. This includes advancing fundamental research in AI algorithms and techniques, developing specialized AI tools and platforms for chemical applications, and providing training and education to empower the workforce to harness the full potential of AI-driven technologies. In conclusion, Artificial Intelligence stands as a powerful catalyst for the chemical industry. By harnessing AI-driven technologies, we can optimize processes, create safer work environments, speed up innovation, streamline supply chains and help facing the challenges of the chemical industry. As AI capabilities continue to improve, the potential for innovation and sustainability could be immense and I am looking forward to seeing these developments.

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