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when using hte to optimize chemical reactions it is important to not only consider the practicalities of how to perform multiple reactions in tandem but also how to analyze and deconvolute the reaction outcome in a similarly high throughput manner

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this review highlights the basics and the cutting edge of modern chemical reaction optimization as well as its relation to process scale up and can thereby serve as a reference for inspired scientists for each of these techniques detailing several of their respective applications go to 1 introduction

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chemical reaction design and optimization is vital in organic synthesis research by altering the reaction parameters catalyst ph solvent temperature or time certain outputs cost savings purity selectivity or yield can be achieved

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deep reinforcement learning was employed to optimize chemical reactions our model iteratively records the results of a chemical reaction and chooses new experimental conditions to improve the reaction outcome

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an efficient and effective framework to optimize chemical reactions will be of great importance for both academic research and industrial production we present here one potential approach to achieving this goal

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machine learning ml techniques applied to chemical reactions have a long history the present contribution discusses applications ranging from small molecule reaction dynamics to computational platforms for reaction planning

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robotic platforms for chemistry are developing rapidly but most systems are not currently able to adapt to changing circumstances in real time we present a dynamically programmable system

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optimize chemical reactions our model iteratively records the results of a chemical reaction and chooses new experimental con ditions to improve the reaction outcome this model out performed a state of the art blackbox optimization algorithm by using 71 fewer steps on both simulations and real reactions

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optimizing chemical reactions is a very common task for chemists it usually aims at maximizing the yield or selectivity of a reaction in order to get the most possible product from some raw material

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machine learning ml is a powerful tool that can be used to optimize chemical processes in chemical engineering ml techniques can be applied to various aspects of process optimization including process modeling process control and process optimization

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in response to the need for efficient optimization of complex photocatalytic reaction conditions we have developed a robotic platform named robochem robochem facilitates the self optimization intensification and scale up of photocatalytic transformations

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process design and optimization is an essential discipline for anyone working in the chemical industry it involves understanding the chemical reaction mechanism designing the plant or refinery for optimal production and optimizing processing conditions to achieve maximum efficiency

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a chemical engineer applies principles of chemistry physics biology and mathematics to design develop and optimize processes and products involving chemical reactions or transformations

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to reach improvements in these performance indicators and optimize chemical conversions enzyme engineering has been developed as one of the pillars of synthetic biology 2 realizing enzyme

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industrialized chemical production is a complex process that requires continuous optimization artificial intelligence has the potential to revolutionize chemical manufacturing learn how ai can improve yields reduce waste and emissions or optimize energy usage

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the ultimate goal of this study is to rapidly determine suitable conditions given reactions with predefined search space optimizing reaction conditions is the process of exploring various

types of reaction parameters such as reagent solvent base catalyst concentration and temperature

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