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Optimal Reuse of Flowback Wastewater in Hydraulic Fracturing Including Seasonal and Environmental Constraints

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This article presents a mathematical programing formulation for the optimal management of flowback water in shale gas wells. The formulation accounts for the time-based generation of the flowback water, the options for treatment, storage, reuse, and disposal. The economic and environmental objectives are considered. The economic objective function is aimed at determining the minimum cost for the fresh water, treatment, storage, disposals, and transportation. The environmental objectives account for the fresh water usage and wastewater discharge. To carry out the water integration, a reuse network including treatment is proposed. Additionally, the model considers seasonal fluctuations in the fresh water availability. A given scheduling for the completion phases of the wells is required to implement the methodology. Finally, an example problem is presented to show the applicability of the proposed methodology. © 2016 American Institute of Chemical Engineers *AIChE J*, 62: 1634–1645, 2016
Keywords: water management optimization, shale gas, hydraulic fracturing (fracking), flowback water reuse, fresh water restrictions

Introduction

Recently, there have been substantial discoveries of shale gas reserves in North America. Hydraulic fracturing technologies have facilitated the production of shale gas trapped in tight formations. According to the Energy Information Administration (EIA), by the year 2035 shale gas is expected to provide about half of the total natural gas supply in the United States.[1] The EIA also estimates that the United States has enough natural and shale gas to meet domestic electricity demands for 575 years at current electricity generation levels. Certainly, this information highlights the importance and the enormous potential of shale gas in the future. Siirola[2] analyzed the impacts of shale gas in the chemical industry and in the natural gas market. Weijermars[3] modeled the future gas production up to 2025 in the six major shale plays of United States under uncertain conditions with the purpose of determining different scenarios of production. Cafaro and Grossmann[4] presented a model to plan the shale gas supply and to determine the number of wells, the size of gas processing plants, the section and length of pipelines for gathering raw gas and delivering processed gas and by-products, the power of gas compressors, and the amount of freshwater required from reservoirs for drilling and hydraulic fracturing so as to maximize the net present value of the project. He and You[5] integrated the shale gas processing with ethylene production to increase the profitability. Yang et al.[6] developed a new design to integrate an oil shale refinery with reforming retorting gas; this scheme allows the production of the required hydrogen in the hydrogenation step and considerable economic benefits are obtained compared with the conventional refinery process. Wang and Xu[7] proposed a new methodology for the simultaneous operation of shale gas, NGL recovery, and LNG re-gasification considering the uncertainty of the shale gas feed rate. Knudsen et al.[8] presented a mathematical formulation for well scheduling using a Lagrangian relaxation. Pirzadeh et al.[9] carried out a study for hydraulic fracturing additives, which are capable of generating H_2S under hydrothermal conditions or delaying the production of native H_2S. Furthermore, He and You[10] presented a novel process design for a greener chemicals production integrating shale gas with bioethanol dehydration and Gao and You[11] designed and planned shale gas supply chains under uncertainty including the drilling, production, processing, and transportation.

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Effect of the anatase–rutile contact in gas phase toluene photodegradation quantum efficiency

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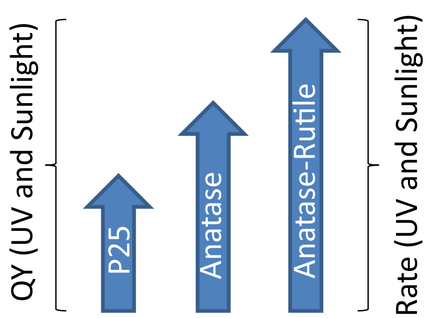
HIGHLIGHTS

- Microwave, calcined titania samples were tested under UV/Sunlight.
- Focus on the catalytic role of the anatase–rutile interface.
- Analysis of activity by means of the quantum efficiency parameter.
- Quantitative assessment of all physical variables of the efficiency parameter.
- Optimum enhancement: synergetic interplay between light-matter and chemical variables.

GRAPHICAL ABSTRACT



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ABSTRACT

A series of TiO_2 samples prepared by a microwave assisted method followed by spray drying and calcination were tested in gas-phase photodegradation of toluene under UV and Sunlight-type illumination conditions. Samples were characterized using X-ray diffraction, porosimetry, UV–visible and photoluminescence spectroscopies as well as transmission and scanning microscopies. Their photochemical behavior was analyzed through their reaction rate and efficiency parameters, the later measured as both the apparent and true quantum efficiency. To interpret photocatalytic properties we carried out a study of the main physico-chemical variables affecting photoactivity and particularly its measurement through the efficiency parameter. In particular we focus on quantifying the catalytic effect of the anatase–rutile interface with respect to a parent anatase material prepared at different calcination temperature and in interpreting quantitatively such enhancement using the above mentioned physico-chemical analysis of the efficiency parameter. The study shows that there are some counteracting physical effects in the toluene photodegradation true quantum efficiency presented by anatase–rutile samples with respect to parent anatase counterparts.

1. Introduction

Since the early days in the photocatalytic field, it was clear that the titania semiconductor displayed the best general performance due to its versatility in photo-degradation and photo-production reactions concerning the elimination or transformation of both

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Enhanced photocatalytic activity of MWCNT/TiO_2 heterojunction photocatalysts obtained by microwave assisted synthesis

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ABSTRACT

Herein reported are the synthesis and the photocatalytic activity of MWCNT/TiO_2 heterojunction photocatalysts obtained by microwave-assisted method using titanium butoxide as precursor. The obtained materials were characterized by XRD, Raman, SEM, TEM, UV–vis, FTIR, surface area (BET) and photoluminescence. The characterization results showed that the addition of MWCNT did not provide structural changes on TiO_2. The photocatalytic activities of the synthesized materials were investigated using acid blue 9 dye as a model molecule. The results indicate an enhancement on photocatalytic activity by the addition of low amount of MWCNT (1 and 3 wt%). The improvement is attained to the synergic effect between TiO_2 and MWCNT which reduces the electron–hole pair recombination according with the photoluminescence study. In this way, a proposed schema for the enhanced photoactivity of the MWCNT/TiO_2 heterojunction photocatalyst is discussed.

1. Introduction

Toxic, recalcitrant, and/or dyed organic compounds can be eliminated by various advanced oxidation processes. They are based on reactive oxygen species (ROS) production as hydroxyl radicals ($OH^{\bullet}$), which are effective for organic contaminants degradation [1]. The production of ROS in heterogeneous photocatalysis is based on the irradiation of semiconductors. The preferred semiconductor used in photocatalysis is titanium dioxide (TiO_2) [2–4], due to its chemical stability, superhydrophilicity, long durability, non-toxicity and low cost [5]. Unfortunately, the rapid recombination of photogenerated electron–hole pairs in the bulk semiconductor decreases the efficiency of photocatalytic reactions [6,7]. Several attempts have been made to increase the photocatalytic activity of semiconductors such as: controlling the morphology and crystal phase; doping with transition metals or nonmetal elements; or coupling with secondary semiconductors/conductors [6,8–10]. Unfortunately, these methods involve compounds that are either thermally unstable, difficult to modify or even toxic. Another possible approach is by coupling TiO_2 with multiwall carbon nanotubes (MWCNTs), which provide a synergistic and cooperative effect that leads to enhancement of the overall photocatalytic performance [6,7,9,11]. In this regard, the improvement is attributed to the enlarged absorption region of TiO_2, the increment of surface area and the enhancement of electronic transfer; therefore, a reduction of electron in the TiO_2 bulk is achieved [12–15]. Different synthesis methods have been used to obtain the TiO_2–MWCNT materials (composites, hybrids, heterojunctions) [3,7,9,16–19]. Nevertheless, most of these methods require long preparation times (several hours or a day), involve multiple steps and have high thermal costs, which often result in structural damage in the MWCNT [14,15]. Moreover, microwave assisted synthesis is a novel technique that offers several advantages, such as simple and fast synthesis procedures, reduces the reaction time, offers faster kinetics, higher yield, uniform heating and minimal structural damage [20,21]. This method has been widely used to obtain pure TiO_2; nevertheless, there are few reports where microwave

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Gas phase 2-propanol degradation using titania photocatalysts: Study of the quantum efficiency

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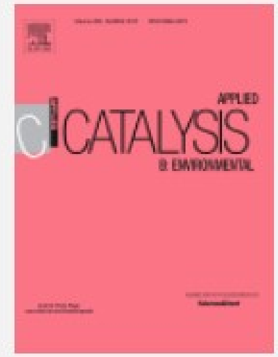

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Abstract

A series of TiO_2 samples, prepared by a microwave assisted method followed by spray drying and subjected to further calcination, were tested in gas-phase photodegradation of 2-propanol under UV and Sunlight-type illumination conditions. Samples were characterized using X-ray diffraction, porosimetry, UV–vis and Photoluminescence spectroscopies. This physico-chemical characterization was completed with the in-situ analysis of the sample behavior under illumination conditions using infrared spectroscopy. The photochemical behavior of the samples was analyzed through their reaction rate and particularly efficiency parameters, the later measured as both the apparent and true quantum efficiency. To calculate the efficiency in quantitative basis we carried out a complete analysis of th...

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Optimal Synthesis of Refinery Property-Based Water Networks with Electrocoagulation Treatment Systems

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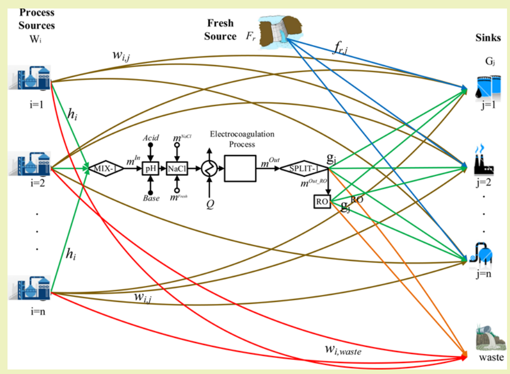
Supporting Information

ABSTRACT: This paper presents an optimization approach to the incorporation of electrocoagulation in the design of integrated water networks for oil refineries. A disjunctive programming formulation is developed to minimize the cost of the water-management system while including the characteristics of process water streams, recycle, reuse, and treatment of wastewater streams, performance of candidate technologies, and composition and property constraints for the process units and the environmental discharges. The performance of electrocoagulation was related to temperature pH and the concentration of phenols and sodium chloride. Ancillary units including pH adjustment, reverse osmosis, and heat exchangers were used to support the electrocoagulation unit. Two case studies are presented to show the applicability of the proposed model and the feasibility of using electrocoagulation as part of an integrated water management scheme for oil refineries.



KEYWORDS: *Electrocoagulation, Recycle and reuse water networks, Optimization, Removal of phenolic compounds, Refinery wastewater*

■ INTRODUCTION

Industrial processes consume tremendous amounts of fresh water and discharge significant quantities of wastewater. Efficient mass-integration strategies that include conservation, treatment, recycle, and reuse are instrumental in reducing water usage and discharge and in abating the environmental impact associated with the discharge of pollutants to water bodies. Three mass-integration approaches have been developed for the design of industrial water networks: graphical (pinch), algebraic, and optimization techniques. For recent reviews, the reader is referred to the works by El-Halwagi and Foo,[1] Klemeš,[2] El-Halwagi,[3] Poplewski,[4] and Foo.[5] Pinch-based methods provide valuable visualization-based understanding of the design of recycle/reuse networks but are limited in terms of scope and size of the problem. On the other hand, mathematical programming techniques can address significantly more complex problems but require specialized knowledge to formulate and solve. A particularly important class of water networks involves the design based on a property integration framework. Property integration is a technique which is based on optimizing the allocation and manipulation of streams to units based on properties. Shelley and El-Halwagi[6] proposed a property-based componentless approach to process integration and introduced the concept of property clusters that can be tracked in a conservative manner. El-Halwagi et al.[7] presented a rigorous graphical targeting approach to minimize the use of fresh resources by using segregation, mixing, and direct recycle/reuse strategies. This approach was revised by Kazantzi and El-Halwagi[8] and Kazantzi et al.[9] to characterize streams and units based on properties through graphical techniques and by Qin et al.[10] and Almutlaq and El-Halwagi[11] through algebraic techniques. El-Halwagi et al.[12] presented new systematic rules and visualization techniques for the identification of optimal mixing of streams and their allocation to units. Furthermore, they presented a derivation of the correspondence between clustering tools and fractional contribution of streams to minimize the usage of fresh resources. Eljack et al.[13] developed property clustering techniques for the simultaneous design of molecular and process networks. Grooms et al.[14] further introduced a source–interception–sink representation to embed structural configurations of interest. Foo et al.[15] introduced two new tools: the property surplus diagram and the property cascade analysis technique to establish rigorous targets on the minimum usage of fresh resources, maximum direct reuse, and minimum waste

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