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Mixing regime simulation and cellulose particle tracing in a stacked frame photocatalytic reactor

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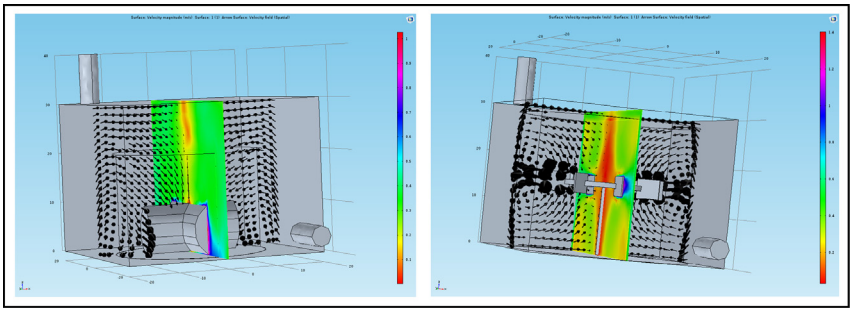
HIGHLIGHTS

- A novel reactor for photocatalytic cellulose breakdown was designed.
- Eight blade Rushton impeller was compared against a stirrer bar.
- Mixing regime and particle tracing simulations were performed using COMSOL.
- Particle tracing simulations confirmed the superiority of the Rushton impeller.

GRAPHICAL ABSTRACT



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ABSTRACT

To sustainably meet the global energy demand, unconventional methods to produce renewable energy must emerge. Biofuels from cellulose (via fermentable sugar production) mediated via photocatalysis provides an alternative to conventional fossil fuels. In order to effectively drive photocatalytic processes an effective reactor design is required, the design of which is influenced by a number of key factors such as the catalyst to reactant ratio and residence time, catalyst illumination time, light penetration and distribution for the system, mass transfer limitations (mixing) and product recovery. In this study we use COMSOL Multiphysics® to simulate and assess one of the mentioned parameters – mixing regime of cellulose particles in a Stacked Frame Photocatalysis Reactor (SFPR). In the reactor design, we compare two mixers: a 'plus' shaped magnetic stirrer bar and an 8 blade Rushton impeller. The simulations reveal that the Rushton impeller offers a radial mixing pattern with a higher fluid velocity of 1.2 m/s when compared to the stirrer bar that offers a fluid velocity of 0.9 m/s. Cellulose particle tracing simulations confirm that the particle dispersion is superior in the case of the Rushton impeller as the vorticity generated during the mixing push the particles to the reactor's walls. Since the particles are forced towards the walls, there is a probability of more particles being illuminated than in the case of no or improper mixing.

1. Introduction

Fossil fuel depletion and raising greenhouse gas emissions have increased the need for alternative renewable energy technologies. Along with solar energy, wind energy and tidal energy, biofuels

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could also contribute to the global clean energy production. Biofuel production could be brought about from various sources such as waste vegetable oil, food waste, animal fats, algae and cellulose. Among these sources, cellulose is the most attractive raw material as it is the world's most abundant organic material [1]. However, cellulose as such cannot be used directly as a fuel and has to be converted to fermentable sugars which can then lead to the production of bio alcohols via fermentation. Conventionally, cellulose hydrolysis has been achieved through environmentally unfavourable, high energy consuming physico-chemical methods such as steam explosion, pyrolysis or acid/alkali hydrolysis [2]. A potential new route for cellulose breakdown using photocatalysis could be an alternative, more sustainable method to breakdown the cellulose molecule to smaller carbohydrate species [3]. Photocatalysis is a light driven chemical reaction. When light of a specific wavelength with energy greater than or equal to band gap energy illuminates a photocatalyst, an electron from the valence band (VB) gets promoted to the conduction band (CB) leaving behind a positive hole in the VB. These positive holes react with water or OH^- to form hydroxyl radicals which can carry out oxidation reactions such as break down of cellulose.

Conventional reactors for chemical engineering are well established and classified, whereas photocatalytic reactor designs are relatively new [4]. In addition to the conventional reactor design parameters such as reactor geometry, mixer configuration, mode of operation (continuous or batch), separation efficiency, residence time, reaction selectivity, materials of construction and cost, the following parameters with respect to illumination need to be considered while designing a photocatalytic reactor [5],

(i) Type of illumination source
(ii) Output power of the light source
(iii) Spectral distribution
(iv) Maintenance
(v) Inclusion of reflectors, mirrors and windows
(vi) Construction materials to facilitate light transmission

Furthermore, the illumination source also influences the choice of materials for reactor construction. When external ultraviolet (UV) light sources are used for photocatalysis, expensive fused silica (quartz) is the primary choice of material for the reactor vessel as standard glass is not fully transparent to UV radiation, especially at wavelengths less than 400 nm. Pyrex glass, which is a cheaper alternative may, however, be used under near UV illumination (350–400 nm) or for visible light photocatalysis. When illumination sources are deployed within the reactor, the unit is made of materials such as aluminium or stainless steel (for reflection and light distribution), however Pyrex or quartz lamp housing units will still be required. A range of light sources that could be used to illuminate the TiO_2 photocatalytic system is summarised in Table 1. In addition, sample spectra of two commonly used UV lamps (500 W Xenon lamp and 36 W fluorescent UV lamps) are shown in Fig. 1.

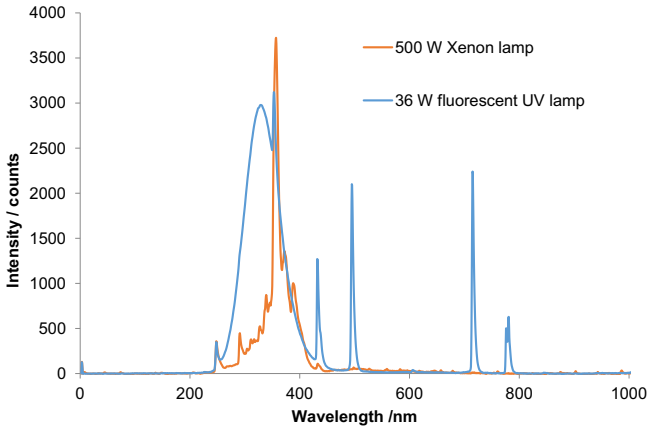

Fig. 1. Lamp spectra of a 500 W Xenon lamp and a 36 W fluorescent UV lamp.

As previously reported in the literature, photocatalytic reactor designs can potentially fulfil the following objectives: [6–8]

(i) Improve the catalyst to reactant ratio and residence time,
(ii) Increase the catalyst illumination time,
(iii) Improve light penetration and distribution for the system,
(iv) Eliminate mass transfer limitations and
(v) Increase the product production and recovery.

Photocatalytic reactors can be broadly grouped under either suspended or immobilised photoreactors based on the mode of photocatalyst deployment. It is not feasible to compare the current reactor designs on a common scale as they have their own advantages and disadvantages based on their area of application [4]. Recently, however, 12 different photocatalytic reactors for wastewater treatment were compared using a benchmark ratio proposed as the photocatalytic space time yield (PSTY) [6]. According to Leblebici et al. PSTY is defined as "the volume of water treated for each kW lamp power per volume of reactor per unit of time" [6]. After normalising various designs using PSTY, they concluded that the pilot scale slurry reactor with a suspended photocatalyst system outperformed the other designs. This was as a result of issues such as high light distribution, decreased mass transfer limitation and high photocatalyst surface area available for illumination and hence is also the most commonly used reactor design in the field of photocatalysis [9,10].

Simulation is a useful tool to compare various reactor configurations or to compare different modifications done to the same reactor design without having to fabricate the actual unit thereby making it a useful tool in engineering design to reduce the time and costs. There are numerous software packages available for such simulations including MATLAB®, ANSYS®, COMSOL Multiphysics®, and SOLIDWORKS®. The rotating machinery turbulent flow k-ε model in COMSOL Multiphysics® 5.1 was used in this

Table 1
Potential illumination sources.

Type of illumination source	Spectral range	Power	Reference
Mercury arc lamp	UV and visible (265–580 nm)	300 W	[28]
Medium pressure mercury arc lamp	UV (peak at 365 nm)	700 W	[29]
Incandescent lamps	UV and visible (200–600 nm)	200 W	[30]
Mercury vapour fluorescent lamp	UV (peak at 254 nm)	6–10 W	[31–33]
PL-L-40 Philips UV lamps	UV (peak at 365 nm)	40 W	[34]
Blacklight blue Panasonic Fluorescent lamps	UV (300–400 nm)	4 W	[35]
Light emitting diodes (FoxUV™)	UV (peak at 360 nm)	454 μW	[36,37]
InGaN Light emitting diodes	UV (390–410 nm)	10–20 mW	[38]
TG Purple Hi LED E1L5M-4P0A2-01 Light emitting diodes	UV (peak at 383 nm)	20 mW	[39]