



Opinion



# Defining Key Performing Indicators for Economically Feasible H<sub>2</sub>O<sub>2</sub> Production by Means of Photocatalysis

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**Abstract:** Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is an important chemical commodity. Currently, the anthraquinone auto-oxidation (AO) process is the dominant method for producing hydrogen peroxide worldwide. However, alternative generation methods are being extensively investigated, most notably photocatalytic H<sub>2</sub>O<sub>2</sub> synthesis. State-of-the-art heterogeneous photocatalysts can now produce H<sub>2</sub>O<sub>2</sub> from water and O<sub>2</sub> with apparent quantum yields (AQYs) of approximately 20% at 420 nm and solar-to-chemical conversion (SCC) efficiencies of several percent. Unlike electrochemical and other emerging methods, photocatalysis can, in principle, deliver H<sub>2</sub>O<sub>2</sub> of high purity, i.e., H<sub>2</sub>O<sub>2</sub> aqueous solution that is free of electrolytes and other foreign species. However, in the efforts of optimizing the structure of photocatalysts and achieving higher AQY, SCC and the yield rate of H<sub>2</sub>O<sub>2</sub> (mol[H<sub>2</sub>O<sub>2</sub>] g<sup>-1</sup>[photocatalyst] h<sup>-1</sup>), the community appears to drift away from another key performing indicator (KPI), which is exceptionally important to make photocatalysis competitive not only to other emerging methods, but also the AO process. This KPI is concentration of H<sub>2</sub>O<sub>2</sub> achieved in photocatalysis. This quantity is still in the range of few millimoles per liter (mM). In this opinion article, we articulate importance of this KPI and the viable, in our opinion, strategies of increasing this value by means of heterogeneous photocatalysis.

**Keywords:** hydrogen peroxide; photocatalysis; solar-to-chemical conversion efficiency; quantum yield; concentration; heterogeneous catalysis

## Introduction

Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is an important chemical commodity, used primarily as a bleaching agent and oxidant. These applications impose specific requirements on its concentration: it must be at least 3 wt.% in aqueous solution. H<sub>2</sub>O<sub>2</sub> aqueous solution of such concentration is typically sold in pharmacies and used as a disinfectant. Anthraquinone auto-oxidation (AO) process is the major method of hydrogen peroxide production, which involves two chemical reactions [1]. In the first step, 2-alkylanthraquinone is hydrogenated over Pd/Al<sub>2</sub>O<sub>3</sub> catalyst to form 2-alkylanthrahydroquinone (Figure 1). In the second step, 2-alkylanthrahydroquinone reacts spontaneously with O<sub>2</sub>, yielding H<sub>2</sub>O<sub>2</sub> and recovering 2-alkylanthrahydroquinone. Typically, hydrogen (H<sub>2</sub>) for the first step is generated from steam methane reforming, which is an energy intensive process. As a result, production of 1 kg of H<sub>2</sub>O<sub>2</sub> requires an input of 2.9–5.7 MJ of energy [2]. Also, it was calculated that production of 1 kg of H<sub>2</sub>O<sub>2</sub> emits 1.33 kg of CO<sub>2</sub> (the CO<sub>2</sub> footprint) [3].

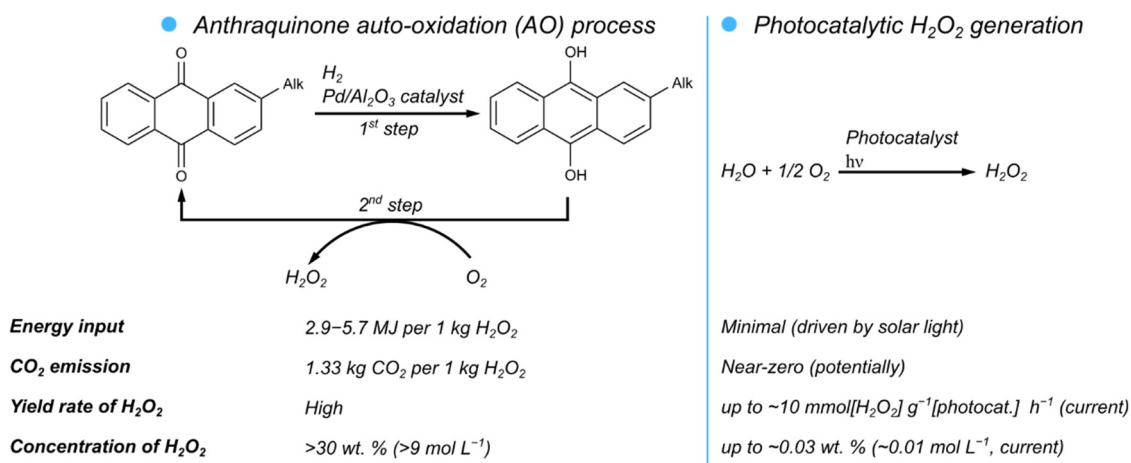
Driven by the necessity to develop more sustainable methods for synthesis of this important chemical, direct synthesis of H<sub>2</sub>O<sub>2</sub> (DSHP), electrochemical, bioelectrochemical, plasmatic and photocatalytic methods, are being investigated actively. These alternative technologies for H<sub>2</sub>O<sub>2</sub> production and their techno-economic feasibility



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were summarized and discussed by Theofanidis and colleagues [2]. Briefly, direct synthesis of H<sub>2</sub>O<sub>2</sub> (DSHP) considers reacting H<sub>2</sub> with O<sub>2</sub> over the noble metal catalyst according to the reaction equation  $H_2 + O_2 \rightleftharpoons H_2O_2$ . If H<sub>2</sub> for this reaction is generated from the renewable source and using renewable energy, the DSHP could become a more sustainable alternative to the AO process. However, this appealing idea is complicated by a number of other thermodynamically and kinetically favorable reactions, such as  $H_2 + 1/2O_2 \rightleftharpoons H_2O$ ,  $H_2O_2 + H_2 \rightleftharpoons 2H_2O$ , which, naturally, decrease the selectivity of H<sub>2</sub>O<sub>2</sub>. In the electrochemical H<sub>2</sub>O<sub>2</sub> synthesis, the desired two-electron water oxidation reaction (more thermodynamically challenging) competes with the undesirable four-electron water oxidation reaction (more thermodynamically favorable). A common feature of DSHP, electrochemical and bioelectrochemical methods is that to achieve viable concentration of H<sub>2</sub>O<sub>2</sub>, for example, 5 wt.% [2], organic solvents, such as decane-1-ol [4], methanol [5], or certain organic additives are required [6]. As a result, an additional step would be necessary to separate H<sub>2</sub>O<sub>2</sub> from organic solvent (similar to the AO process) to deliver H<sub>2</sub>O<sub>2</sub> to the end users.



**Figure 1.** Comparison of the AO process and the photocatalytic H<sub>2</sub>O<sub>2</sub> generation in terms of energy input, CO<sub>2</sub> footprint, yield rate and concentration of H<sub>2</sub>O<sub>2</sub>.

Compared to the discussed above DSHP, electrochemical and bioelectrochemical methods, the state-of-the-art photocatalytic systems are free of noble metals [7,8]. While the discussed above methods could utilize solar energy through a series of converters, a solar panel (and a battery), photocatalysis is driven by the solar light directly. This feature minimizes potential losses of energy upon conversion of the electromagnetic radiation in the UV-vis-nIR range of the spectrum into the electromotive force.

Analysis of the work done in the field of photocatalytic H<sub>2</sub>O<sub>2</sub> generation indicates that the community works primarily in two directions: (1) H<sub>2</sub>O<sub>2</sub> generated photocatalytically using (organic) sacrificial electron donors, such as alcohols [9], and (2) H<sub>2</sub>O<sub>2</sub> generated photocatalytically from water only (or water and O<sub>2</sub>). In the first approach, the counterproductive recombination of photogenerated carriers is suppressed by employing sacrificial electron donors [10]. As such, the efficacy of two-electron O<sub>2</sub> reduction to H<sub>2</sub>O<sub>2</sub> is maximized. However, from the practicality standpoint of H<sub>2</sub>O<sub>2</sub> generation via this approach, it does not solve the problem of reliance on organic solvents and additives, which is similar to DSHP and electrochemical methods, and yields a mixture of H<sub>2</sub>O<sub>2</sub> and organic species in water. Unless, oxidation of electron donor and reduction of O<sub>2</sub> are decoupled in time [11] (and space as in “dark” photocatalysis [12–14] which conceptually would be similar to the AO process), photocatalysis, in this scenario, produces a complex mixture of species, which application is limited.

The second photocatalytic approach is definitely more appealing. Provided that the employed photocatalyst is heterogeneous, it may be separated easily from the liquid phase while affording aqueous solution of H<sub>2</sub>O<sub>2</sub> which concentration depends on the activity of the employed photocatalyst and the process parameters. Further analysis of published data indicates that the community focuses largely on optimizing the yield rate of H<sub>2</sub>O<sub>2</sub> (mol[H<sub>2</sub>O<sub>2</sub>] g<sup>-1</sup>[photocatalyst] h<sup>-1</sup>), apparent quantum yield (AQY, % at certain wavelength) and the solar-to-chemical conversion (SCC, %) efficiency [15]. Figure 2 summarizes these metrics, their advantages and limitations. A growing number of publications apply the SCC metric to reactions characterized by a negative  $\Delta_r G^0$  value, such as the spontaneous production of H<sub>2</sub>O<sub>2</sub> via O<sub>2</sub> reduction using benzyl alcohol as a sacrificial electron donor,  $PhCH_2OH + O_2 \rightleftharpoons PhC(O)H + H_2O_2$ . In such spontaneous processes, solar energy is not converted into the potential energy of chemical bonds. We wish to emphasize that the SCC metric should be reserved exclusively for reactions

with a positive  $\Delta_r G^0$  value—those that are non-spontaneous in the dark—such as the direct synthesis of  $H_2O_2$  from water and oxygen (Figure 2).

### ● Metrics

**Apparent quantum yield (AQY)** – A fraction of photons of specific wavelength that mediates formation of  $H_2O_2$

$$AQY = \frac{n(H_2O_2)}{n(\text{photon})} \times 100\% \quad (\text{at certain wavelength})$$

- + Applicable to any photocatalytic reaction that yields  $H_2O_2$ , i.e. using  $H_2O$  (and  $O_2$ ) as well as organic sacrificial electron donors
- + Characterizes photocatalyst's efficacy at specific wavelength

**Solar-to-chemical conversion (SCC) efficiency** – A fraction of solar radiation energy that is stored in  $H_2O_2$

$$SCC = \frac{\Delta_r G^0 \times n(H_2O_2)}{P \times S \times t}$$

- + Applicable and should be used only for endergonic reactions ( $\Delta_r G^0 > 0$ )
- + Grasps the efficacy of the photocatalyst to utilize solar light
- Reaction equation describing  $H_2O_2$  synthesis must be known to calculate  $\Delta_r G^0$

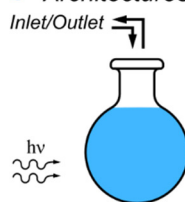
**$H_2O_2$  production rate (r)** – Productivity of a photocatalyst

$$r = \frac{n(H_2O_2)}{m(\text{photocat.}) \times t}$$

- + Applicable for any (photo)catalytic reaction – allows for comparison of photocatalysts' productivity with the productivity of thermal catalysts

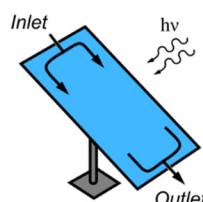
$n(H_2O_2)$  – amount of produced  $H_2O_2$ , mol.  
 $n(\text{photon})$  – amount of emitted photons, mol.  
 $\Delta_r G^0$  – standard Gibbs free energy change in the reaction of  $H_2O_2$  synthesis, such as  $H_2O + 1/2O_2 = H_2O_2$ , J mol<sup>-1</sup>.  
 $P$  – solar radiation power at 1.5 atmospheric masses, 1000 W m<sup>-2</sup>.  
 $S$  – area of the photoreactor, m<sup>2</sup>.  
 $t$  – reaction time, s.  
 $m(\text{photocat.})$  – mass of the photocatalyst, g.

### ● Architectures of photoreactors



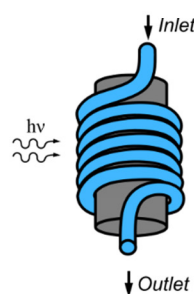
#### **Batch photoreactor:**

- + Simplest design → available in every laboratory
- Poor light delivery into the bulk of the reaction mixture
- Large solvent volume → low  $H_2O_2$  concentration
- ...



#### **Thin-film photoreactor:**

- + Light delivery is the most efficient
- Requires specialized equipment for photocatalyst deposition (dip coating, spray coating, etc.)
- Delamination of the photocatalyst from the supporting surface
- ...

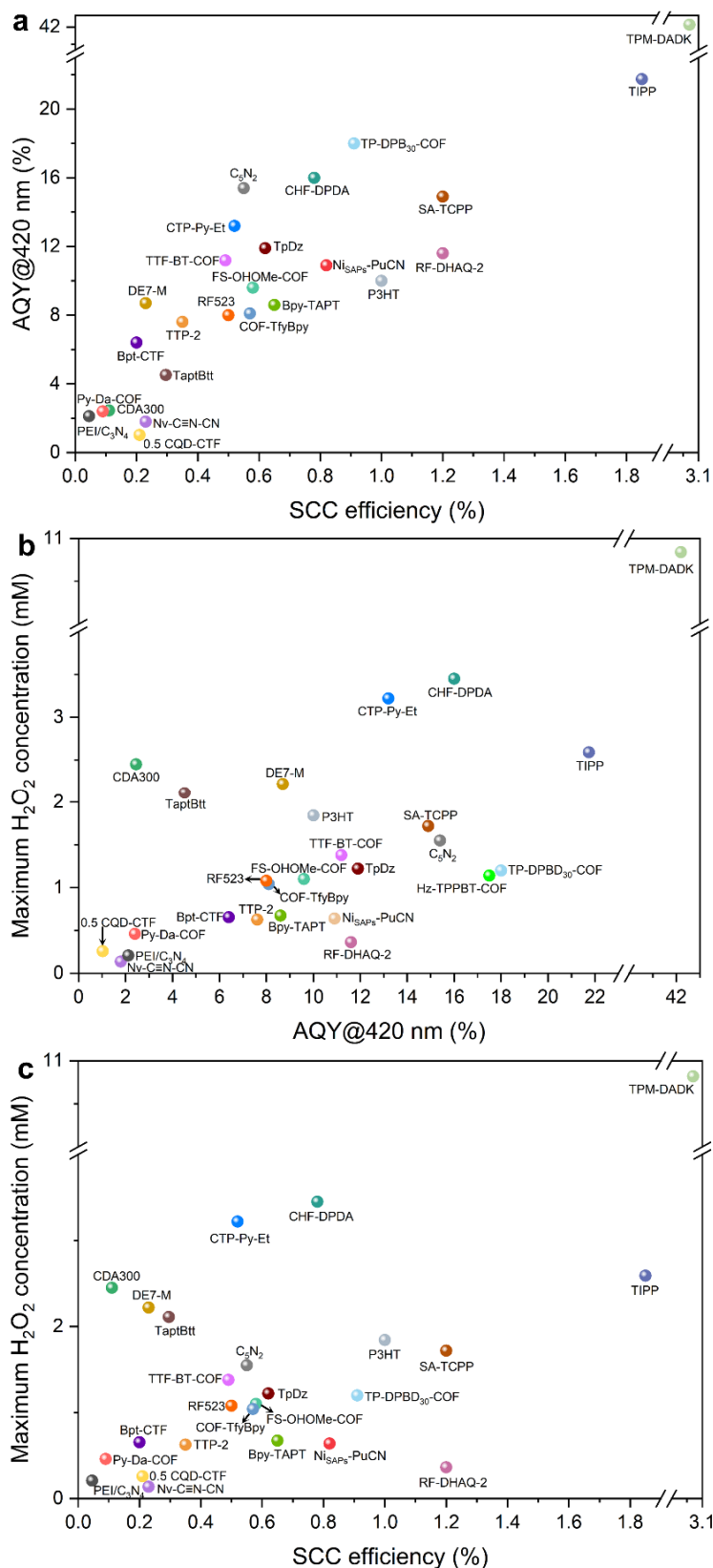


#### **Continuous flow photoreactor:**

- + Concentration of  $H_2O_2$  scales reversibly with the flow rate
- + High back-pressure → high concentration of  $O_2$  in liquid phase → higher rate of  $H_2O_2$  production
- Requires specialized equipment
- High back-pressure → high hydrodynamic resistance
- ...

**Figure 2.** Comparison of performance metrics for photocatalysts, alongside the advantages and limitations of three photoreactor architectures.

Until now, the AQY values greater than few tens percent at 420 nm [7,16], and the SCC of >3% were achieved, which is encouraging [17–19]. These metrics are exceptionally important for developing high-performing photocatalysts. And there is definitely a room for improvement by creating intrinsically more active photocatalysts, which would afford greater AQY and the SCC. Given that  $H_2O_2$  is primarily used as a bleaching agent and oxidant, achieving higher concentration during the photocatalytic experiments is essential for making these methods practical. However, a literature analysis suggests that the final concentration of generated  $H_2O_2$  is often treated as a metric of minor significance, as the research community remains largely focused on competing for higher AQY and SCC values. This trend stems partly from the fundamental nature of research in photocatalyst design; although the photocatalysts target synthesis of a major chemical commodity, current research is generally conducted at Technology Readiness Level (TRL) 1 to 2. Because publishing of research data does not require advancing to higher TRLs, the primary focus remains on catalytic activity—quantified via AQY, SCC and the yield rates—rather than the cumulative concentration of  $H_2O_2$ . Consequently, the concentrations achieved via photocatalysis remain significantly lower than those produced by the industrial AO process, and, in many cases, are even lower than those reached through DSHP or photoelectrochemical methods [20].



**Figure 3.** Overview of key performing indicators. (a) Dependence of AQY at 420 nm on SCC efficiency. (b) Dependence of maximum  $\text{H}_2\text{O}_2$  concentration on AQY at 420 nm. (c) Dependence of maximum  $\text{H}_2\text{O}_2$  concentration on SCC efficiency. Articles in which  $\text{H}_2\text{O}_2$  was generated photocatalytically from water and  $\text{O}_2$  are considered. TP-DPBD<sub>30</sub>-COF [15], Hz-TP-BT-COF [16], TPM-DADK [19], FS-OHOMe-COF [21], Nv-C≡N-CN [22], CDA300 [23], COF-TfyBpy [24], RF523 [25], TTP-2 [26], Bpy-TAPT [27], TapItBtt [28], TpDz [29], SA-TCPP [18], CHF-DPDA [7], DE7-M [30], P3HT [31], TTF-BT-COF [32], Py-Da-COF [33], NiSAPs-PuCN [34], PEI/C<sub>3</sub>N<sub>4</sub> [35], C<sub>2</sub>N<sub>5</sub> [36], RF-DHAQ-2 [17], 0.5 CQD-CTP [37], Bpt-CTP [38], TIPP [39]. This figure is adapted from Ref. [8]. Available under a CC-BY 4.0 license. Copyright 2026 Wang et al.

While AQY, SCC are the parameters intrinsic to the photocatalyst, yield rate and especially concentration of  $\text{H}_2\text{O}_2$  may be increased by adjusting the process parameters. Figure 2 summarizes some advantages and limitations of three types of photoreactors. Although batch reactors are characterized by design simplicity, they typically achieve concentrations in the millimolar range within a few hours of the reaction mixture exposure to light. Such relatively low concentrations arise from the interplay between standard reaction volumes (10–50 mL) and observed photocatalytic yield rates ( $0.1\text{--}10 \text{ mmol}[\text{H}_2\text{O}_2] \text{ g}^{-1}[\text{photocatalyst}] \text{ h}^{-1}$ ). Using a transition metal free covalent triazine polymer CTP-Py-Et (Figure 3), Wang and colleagues increased concentration of  $\text{H}_2\text{O}_2$  several times by simple adjustment of reaction volume and the amount of the photocatalyst [8]. Minimizing the water volume, or potentially conducting the photocatalytic reaction in moist  $\text{O}_2$ , could yield  $\text{H}_2\text{O}_2$  in much higher concentrations. Alternatively, flow technology offers superior control over light delivery and reaction volume, which could also facilitate higher  $\text{H}_2\text{O}_2$  concentrations. For example, Guo and colleagues increased  $\text{H}_2\text{O}_2$  concentration by decreasing the flow rate [39].

Nevertheless, challenges of increasing  $\text{H}_2\text{O}_2$  concentration remain—strong light scattering by the suspended particles of semiconductor photocatalyst, which restricts using dispersions of high optical density. Additionally, the light intensity decreases exponentially as it penetrates deeper into the water-photocatalyst mixture, according to the Beer-Lambert law. Therefore, scaling up the process in batch by simply increasing the volume of the reaction mixture is not efficient—only a fraction of photocatalysts particles, dispersed in the thin layer close to the surface of the reactor, is exposed to light and enables the photoredox reaction, while majority of them remain in the dark, in the bulk of the reaction mixture. This results in low efficacy of the catalyst utilization. Promising approaches to overcome this issue include immobilization of the heterogeneous photocatalyst in the form of thin film, switching to the flow technology and increasing the  $\text{O}_2$  concentration by employing backpressure regulators (Figure 2). This can potentially overcome the gas-liquid mass transfer limitation and avoid the additional separation of the catalyst and product ( $\text{H}_2\text{O}_2$ ), which would incur extra cost.

We are strongly convinced that to make  $\text{H}_2\text{O}_2$  production by means of photocatalysis competitive with the AO process and other emerging (potentially more sustainable) methods, efforts should be dedicated to increasing the concentration of  $\text{H}_2\text{O}_2$  in the reaction mixture. The first target could be to achieve  $\text{H}_2\text{O}_2$  concentration of 3 wt.% ( $0.88 \text{ mol L}^{-1}$ ) by employing water and  $\text{O}_2$  as the only reactants. While achieving this goal it is imperative that the photocatalyst maintains its activity over extended operation, is easily recovered from the  $\text{H}_2\text{O}_2$  solution, and can be reused over multiple cycles without significant performance loss. This would render photocatalysis as a viable method of distributed production of  $\text{H}_2\text{O}_2$  for its application as the disinfectant.

### Author Contributions

O.S.: conceptualization, supervision, investigation, writing—original draft preparation; C.W.: data curation, visualization, investigation; Z.Y.: investigation, writing—reviewing and editing; Z.C.: investigation, writing—reviewing and editing. All authors have read and agreed to the published version of the manuscript.

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### Conflicts of Interest

The authors declare no conflict of interest.

### Use of AI and AI-Assisted Technologies

No AI tools were utilized for this paper.

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