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Design of a high-pressure catalytic photorreactor to operate at supercritical CO_2 conditions

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Abstract

Design a chemical reactor is a complex process since it must allow flexible operation in the ranges of temperature and pressure required by the chemical process that is to be developed. Nature of the substances involved, the phases present, the kinetics and thermodynamics of the process are considered. Especially when it comes to photocatalytic reactors since radiation plays a leading role in the reaction process these are aspects of high relevance for the selection of materials, type of operation, fluid dynamics and geometry1,2.

Commercially, we can find reactors built in different materials such as steels, sapphire, borosilicate, PVC, some of these designed to withstand high pressures, others allow lighting inside the reactor, and another group operates in heterogeneous systems with suspended catalysts. However, having these three characteristics in a single device requires a rigorous mechanical analysis and some modifications in the commercial designs of high-pressure reactors3. Due to the expansion that heterogeneous photocatalysis has had in recent decades due to the variety of chemical processes that can be performed. Such as selective oxidation reactions using atmospheric oxygen4,5, where there is a great interest in replacing organic solvents with supercritical fluids, especially CO_2. These high pressure photoreactors are required4. Since the reactors for heterogeneous photocatalysis using scCO2 as a solvent are few and often use immobilized acid catalysts. In this work, a photoreactor was designed to allow processes of transfer of oxygen atoms to olefins using $scCO_2$ as a solvent and a dioxo-molybdenum complex supported on TiO2 as a catalyst, activated by UV-Vis radiation6.

Methodology:

In Fig. 1, the primary considerations for the selection of materials, geometry and couplings for the design of the batch photoreactor are shown. The nature of the substances, the reactions and the operating conditions to which this equipment is subjected. The design rules for high pressure vessels presented in ASME VIII code were used to establish the mechanical requirements for the construction of the high-pressure reactor. These data were simulated and adjusted using the finite element method using the CAD-type software, Solid Work, the main equations used are shown in Table 1.

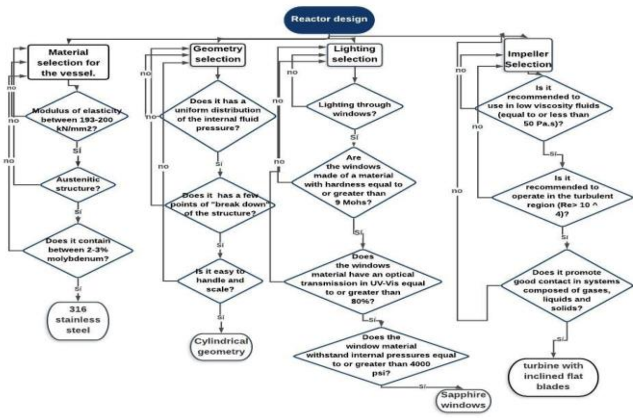

Fig 1. Design criteria for reactor.

Main design equations	
$t=\frac{PR}{SE-0.6P}$	Thickness of the reactor vessel
$H=\frac{\pi*G^2*P}{4}$	Fluid pressure inside the vessel
$H_P=\pi*G*2*m*P*b$	Packing load
$W_{m1}=H+H_p$	Bolt load in service
$W_{m2}=\pi*b*G*y$	Load of bolts in settlement
$A_m=\frac{W_{m1}}{f_a}\ o\ \frac{W_{m2}}{f_b}$	Minimum cross-sectional area of the bolt
$A_b=\frac{\pi}{4}*d_{br}^2*\#\ bolts$	Real diameter of bolt circle

Table 1. Main design equations

Biography:
Estany Pajaro is a student currently pursuing her Masters at Industrial University of Santander in Colombia.

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