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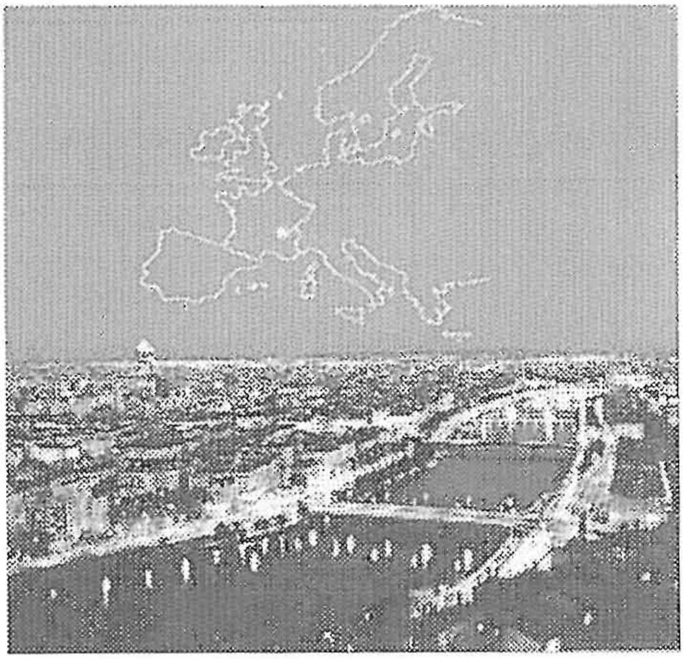

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KINETICS FOR CATALYTIC WET AIR OXIDATION OF BUTYRIC ACID

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Catalytic Wet Air Oxidation (CWAO) is an emerging liquid phase process for treating industrial effluents containing a high Chemical Oxygen Demand. This technology can efficiently degrade organic species provided that a suitable catalyst is used [1].

In this work we used an Ir/C catalyst to study the CWAO of butyric acid solutions. This carboxylic acid was used as a model substrate, due to the refractory nature associated to this low molecular weight type of compounds, which are normally found as end products in the oxidative degradation of most organic species. In addition, the chain length with four carbon atoms allows us to study the oxidation mechanism in more depth. From the catalytic experiments, we concluded that after adsorption of the substrate at the iridium surface, the oxidation reaction proceeds through a hydrogen abstraction step assisted by oxygen reactive species.

The experimental results were modeled considering the reaction scheme presented in Figure 1, where But, Prop and Acet are butyric, propionic and acetic acids, respectively.

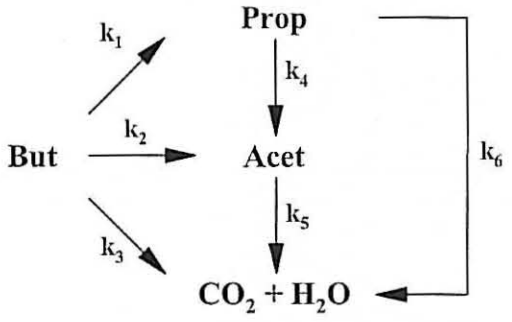

Figure 1 – Reaction scheme for CWAO of butyric acid

The model employed was based on a Langmuir-Hinshelwood mechanism. It was assumed that the reaction occurs at neighbour metal sites, between an adsorbed organic molecule and atomic oxygen (resulting from dissociation after adsorption). Competitive adsorption between all species was also considered. Typical results for butyric acid oxidation over an Ir/C catalyst at 200°C and 6.9 bar of oxygen partial pressure can be found in Table 1.

Table 1 – Results of kinetic modeling

Rate constant ($mmol.h^{-1}.g_{Ir}^{-1}$)						**Adsorption constant ($L.mmol^{-1}$)**			
k_1	k_2	k_3	k_4	k_5	K_6	K_{But}	K_{Prop}	K_{Ace}	K_{O2}
$1.6x10^6$	$3.6x10^6$	$4.7x10^6$	$3.6x10^5$	$1.4x10^5$	$2.1x10^6$	$1.2x10^{-6}$	$4.9x10^{-6}$	$2.4x10^{-5}$	$4.1x10^{-5}$

A good correlation was observed between the model and the experimental results, allowing us to get a deeper knowledge about the oxidation behaviour of this class of compounds.

Acknowledgement - HTG gratefully acknowledges Fundação para a Ciência e a Tecnologia for his PhD grant (PRAXIS XXI/BD/13498/97).

[1] Gomes H.T., Figueiredo J.L., Faria J.L., Applied Catalysis B 2000, 27, L217.