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Theoretical Description for Sunset Yellow Electrochemical Determination in Food, Assisted by Poly(3,4-ethylenedioxypyrrole) – VO(OH) Composite

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Abstract: In this work, the possibility for sunset yellow electrochemical determination, assisted by the composite of VO(OH) with conducting polymer, has been evaluated theoretically. The correspondent balance equation model of three variables has been developed and analyzed by means of linear stability theory and bifurcation analysis. The oscillatory and monotonic instabilities are shown to be manifested more probably than for the simplest case. The double electric layer (DEL) is influenced by the cyclic changes of ionic force observed during ionic forms' chemical transformation. Nevertheless, the CP – VO(OH) composite may be considered an efficient electrode modifier for yellow sunset determination.

Keywords: Sunset Yellow; Sudan dyes; electrochemical sensors; conducting polymers; vanadium (III) oxyhydroxide; stable steady-state

1. Introduction

Sunset yellow (E110) is one of the most used petroleum-derived orange azo-dyes [1-5]. It is a salt of a sulfonic derivative of the Sudan family (Figure 1). It is used in food, condoms, cosmetics, and drugs. Alongside E123 (amaranth), it produces brown coloring of chocolates and caramel.

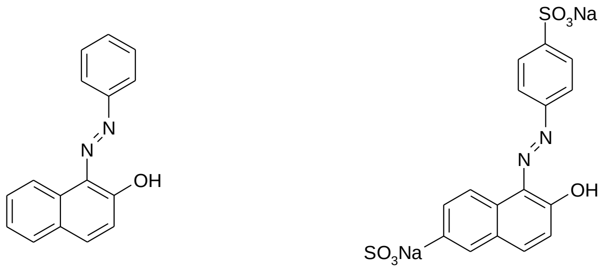

Figure 1. Sudan I (left side) and Sunset Yellow (right side).

The dye's ADI is 0-4 mg/kg both in the EU and the US. While in excess, the dye may be genotoxic, cytotoxic, and carcinogenic [6–8]. Thus, the development of an efficient method for its determination is actual, and the electroanalytical methods could provide a good service [9 - 12].

Sudan dyes constitute a popular object for electroanalytical investigation [13 – 16]. Moreover, possessing both oxidizing or reducing groups, they may be determined by both the cathodic and anodic way. Sunset yellow, as one of the members of the Sudan family, may also be determined by this. In work [17], we have shown that the cathodic determination may provide a more stable and efficient manner to detect Sudan dyes. Therefore, in this work, we evaluate the possibility of the determination of Sunset Yellow (E110), assisted by the composite, in which the conducting polymer poly(3,4-ethylenedioxypyrrole) hosts the active vanadium (III) oxyhydroxide particles.

As both electroanalytical and electro-synthetical processes involving conducting polymers tend to be accompanied by electrochemical instabilities, [18 – 21], influencing the behavior of the electroanalytical process, it is necessary to verify their probability to occur by a theoretical *a priori* analysis, also permitting the theoretical comparison of the electroanalytical system with the similar ones.

Therefore, in this work, the process with sunset yellow electrochemical determination on poly(3,4-ethylenedioxypyrrole) – VO(OH) composite is theoretically evaluated by developing and analyzing the correspondent mathematical model.

2. Materials and Methods

2.1. System and its modeling.

In mildly acidic pH, vanadium (III) oxyhydroxide may be oxidized in two ways:

$$VO(OH) - e^- \rightarrow VO_2 + H^+ \tag{1}$$

$$VO(OH) + 2H^+ - e^- \rightarrow VO^{2+} + H_2O \tag{2}$$

Either vanadium oxyhydroxide or vanadyl are reduced on the electrochemical stage. Therefore, the scheme for the electroanalytical process will be exposed, as in Figure 2.

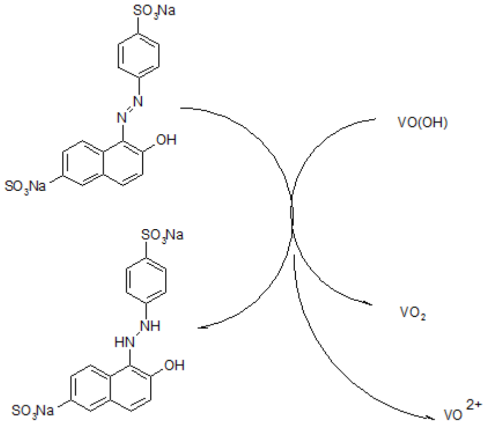

Figure 2. The scheme for the electroanalytical process.

So, in order to describe the behavior of this system, we introduce three variables:

s – Sunset yellow concentration in the pre-surface layer;

v_1 – vanadium (IV) oxide matrix coverage degree;

v_2 – vanadyl-ion matrix coverage degree.

To simplify the modeling, we assume that:

- the background electrolyte is taken in excess so that we can neglect the migration flow and the oxidizing dopant oxidation change;

- the reactor is intensively stirred so that we may neglect the convection flow;

- the pre-surface layer concentration profile is linear, and its thickness is constant, equal to δ.

It is possible to prove that the differential equations´ set, describing the system may be described as:

$$\begin{cases} \frac{ds}{dt} = \frac{2}{\delta}\left(\frac{\Sigma}{\delta}(s_0 - s) - r_{11} - r_{12}\right) \\ \frac{dv_1}{dt} = \frac{1}{V_1}(r_{11} - r_{21}) \\ \frac{dv_2}{dt} = \frac{1}{V_2}(r_{12} - r_{22}) \end{cases} \qquad (3)$$

Herein, Σ is the diffusion coefficient, s_0 is the sunset yellow dye bulk concentration, V_1 and V_2 are maximal matrix concentrations of each of the form of the tetravalent vanadium, and the parameters r are the correspondent reaction rates, which may be calculated as:

$$r_{11} = k_{11}s(1\text{-}v_1\text{-}v_2)\exp(\text{-}as) \qquad (4)$$

$$r_{12} = k_{12}s(1\text{-}v_1\text{-}v_2)\exp(\text{-}as)\exp(bv_2) \qquad (5)$$

$$r_{21}=k_{21}v_1\exp\left(-\frac{F\varphi_0}{RT}\right) \qquad (6)$$

$$r_{22}=k_{22}v_2\exp\left(-\frac{F\varphi_0}{RT}\right) \qquad (7)$$

Herein, the parameters k are the correspondent reaction rate constants, a and b are the parameters relating the double electric layer (DEL) capacitance with the transformation of sunset yellow ionic form and vanadyl ion, F is the Faraday number, φ_0 is the potential slope in DEL, related to the zero-charge potential, R is the universal gas constant, and T is the absolute temperature of the solution.

This system's behavior is more dynamic, as sunset yellow is an ionic compound, and its transformation to another ionic form will give its strong impact to DEL ionic force, structure, and conductivity. Another factor is that one of the tetravalent vanadium forms is charged, so its formation and destruction will also have its strong impact on the system’s behavior. Nevertheless, the system's analysis shows that the electrochemical process will be electroanalytical-efficient, as shown below.

3. Results and Discussion

To investigate the yellow sunset determination, assisted by a hybrid composite of poly(3,4-dimethoxypyrrole) with vanadium (III) oxyhydroxide, we analyze the equation-set (1) employing the linear stability theory and bifurcation analysis. The steady-state Jacobian matrix members for this system will be described as:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{23} & a_{33} \end{pmatrix} \qquad (9)$$

Herein:

$$a_{11} = \frac{2}{\delta}\Big(-\frac{\Sigma}{\delta} - k_{11}(1 - v_1 - v_2)\exp(-as) + ak_{11}s(1 - v_1 - v_2)\exp(-as) - k_{12}\,(1 - v_1 - v_2)\exp(-as)\exp(bv_2) + ak_{12}s(1 - v_1 - v_2)\exp(-as)\exp(bv_2)\Big) \qquad (10)$$

$$a_{12} = \frac{2}{\delta}(k_{11}\exp(-as) + k_{12}\,(1 - v_1 - v_2)\exp(-as)\exp(bv_2)\,) \qquad (11)$$

$$a_{13} = \frac{2}{\delta}(k_{11}\,exp(-as) + k_{12}\,(1 - v_1 - v_2)\,exp(-as)exp(bv_2) - bk_{12}s(1 - v_1 - v_2)\,exp(-as)exp(bv_2)) \quad (12)$$

$$a_{21} = \frac{1}{V_1}(k_{11}(1 - v_1 - v_2)\,exp(-as) - ak_{11}s(1 - v_1 - v_2)\,exp(-as)) \quad (13)$$

$$a_{22} = \frac{1}{V_1}\left(-k_{11}\,exp(-as) - k_{21}\,exp\left(-\frac{F\varphi_0}{RT}\right) - jk_{21}v_1\,exp\left(-\frac{F\varphi_0}{RT}\right)\right) \quad (14)$$

$$a_{23} = \frac{1}{V_1}(-k_{11}\,exp(-as)\,) \quad (15)$$

$$a_{31} = \frac{1}{V_2}(k_{12}\,(1 - v_1 - v_2)\,\mathrm{exp}(-as)\mathrm{exp}(bv_2) - ak_{12}s(1 - v_1 - v_2)\,\mathrm{exp}(-as)\mathrm{exp}(bv_2))\ (16)$$

$$a_{32} = \frac{1}{V_2}(-k_{32}\,\mathrm{exp}(-as)) \quad (17)$$

$$a_{33} = \frac{1}{V_2}\left(-k_{12}\,(1 - v_1 - v_2)\,exp(-as)exp(bv_2) + bk_{12}s(1 - v_1 - v_2)\,exp(-as)exp(bv_2) - k_{22}\,\mathrm{exp}\left(-\frac{F\varphi_0}{RT}\right) - jk_{22}v_2\,\mathrm{exp}\left(-\frac{F\varphi_0}{RT}\right)\right) \quad (18)$$

Taking into account the main diagonal matrix elements (10), (14), and (18), it is possible to conclude that the oscillatory behavior in this system tends to be more probable than in the similar ones [18 – 21], as the ionic forms are transformed in either analyte or an electrode modifier (in the case, vanadyl-ion), leading to the positive callback tendentious, directly linked with the oscillatory behavior.

The positive callback is described by the positive elements in the Jacobian main diagonal. In this system, the elements capable of being positive are:

$ak_{11}s(1 - v_1 - v_2)\,\mathrm{exp}(-as) > 0$ and $ak_{12}s(1 - v_1 - v_2)\,\mathrm{exp}(-as)\mathrm{exp}(bv_2) > 0$ if a>0, describing the positive callback, obtained during the oxidized and reduced Sunset yellow forms ionic transformations. They are cyclic, leading to the cyclic changes in DEL structure, ionic force, and conductivity, defining the oscillatory behavior;

$bk_{12}s(1 - v_1 - v_2)\,exp(-as)exp(bv_2) > 0$, if b>0, describes the analogous cyclic behavior of DEL during the vanadyl formation and destruction;

$-jk_{21}v_1\,exp\left(-\frac{F\varphi_0}{RT}\right) > 0$ and $-jk_{22}v_2\,\mathrm{exp}\left(-\frac{F\varphi_0}{RT}\right) > 0$, if j<0, describing the typical oscillatory factor for the analogous systems, linked to the DEL changes on the electrochemical stages.

Considering that all of the oscillatory factors are linked to DEL and surface conductivity, ionic force, and structure, the oscillation amplitude will be highly dependent on the background electrolyte. Nevertheless, it is realized for the parameter values far beyond the detection limit.

Yet if the above-mentioned conditions aren't satisfied, the steady-state stability requirement is satisfied. To derive it, we apply the Routh-Hurwitz criterion to the equation-set (3), and avoiding the cumbersome expressions, we introduce new variables and rewrite the Jacobian matrix determinant as:

$$\frac{2}{\delta V_1 V_2}\begin{vmatrix} -\kappa - \Xi - \Omega & \Lambda + \mathrm{P} & \mathrm{T} + \Phi \\ \Xi & -\Lambda - \mathrm{G} & -\mathrm{T} \\ \Omega & -\mathrm{P} & -\Phi - \mathrm{E} \end{vmatrix} \quad (19)$$

Opening the brackets and applying the Det J<0 conditions, salient from the criterion, we obtain the steady-state stability requirement, exposed as:

$$-\kappa(\Lambda\Phi + \Lambda\mathrm{E} + \mathrm{G}\Phi + \mathrm{GE} - \mathrm{PT}) - \Xi(\Lambda\Phi + \mathrm{G}\Phi + \mathrm{GE} - \Lambda\mathrm{P} - \mathrm{PE}) - \Omega(\Lambda\Phi + \Lambda\mathrm{E} + \mathrm{GE} - \Sigma\mathrm{T} - \Lambda\mathrm{P}) < 0 \quad (20)$$

Defining either diffusion or kinetically controlled system. The condition (20) is satisfied for a much more narrow topological parameter range than in similar systems [18–21]; nevertheless, this range remains relatively vast. Moreover, as there are no side reactions capable of compromising the modifier(s) or analyte stability, the stable steady-state will always be electroanalytical-efficient.

In other words, the steady-state stability will always correspond to the linearity of the dependence between the electrochemical parameter and concentration, and this linearity will be correspondent to a vast concentration interval.

As for the detection limit, it is correspondent to the monotonic instability. Its point separates the stable steady-states from unstable states, being conditioned to (21):

$$-\kappa(\Lambda\Phi + \Lambda\mathrm{E} + \mathrm{G}\Phi + \mathrm{GE} - \mathrm{PT}) - \Xi(\Lambda\Phi + \mathrm{G}\Phi + \mathrm{GE} - \Lambda\mathrm{P} - \mathrm{PE}) - \Omega(\Lambda\Phi + \Lambda\mathrm{E} + \mathrm{GE} - \mathrm{GT} - \Lambda\mathrm{P}) = 0 \quad (21)$$

Suppose only one of the tetravalent vanadium forms is obtained during the modifying material oxidation. In that case, the third equation will leave the equation-set, transforming it into a bivariant. The system, therefore, becomes analogous to similar ones [18 – 21].

4. Conclusions

The model's analysis lets us conclude that the sunset yellow (E110) dye may be efficiently determined by the vanadium (III) oxyhydroxide with conducting polymer. The oscillatory and monotonic instabilities tend to be more probable than for the simplest case. The double electric layer (DEL) is highly influenced by the transformations of ionic forms, leading to ionic force's cyclic changes. Nevertheless, the steady-state stability is easy to obtain and maintain, so CP – VO(OH) composite is proven to be a suitable electrode modifier for yellow sunset determination.

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Conflicts of Interest

The authors declare no conflict of interest.

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