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CHROMATICITY POINTS OF REAL SPECTRA OUTSIDE THE CIE CHROMATICITY DIAGRAM

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Abstract

When an expert of colorimetry is asked whether the chromaticity point of a real spectrum can fall outside the CIE xy chromaticity diagram, the immediate answer will probably sound like ‘No! This is not possible!’ However, regular spectra generated with a mathematical model function for substituting those of real amber LEDs led to an unexpected fact. Their chromaticity points were close to the boundary, yet outside the CIE xy chromaticity diagram. Deeper investigations discovered that there are several parts of the chromaticity diagram where the concept of convexity is violated. The results have no consequences for most calculations or practical measurements, hence the deviations are only visible in the 5th decimal place. Yet, they may imply a need for revising the colour matching functions, hence an axiom-like property – convexity – of the chromaticity diagram, relevant to the theory of colorimetry, has been disproved.

Keywords: chromaticity diagram, convexity, axiom, LED.

1 Introduction

When somebody claims that they can construct regular spectra – meaning that there are no negative values in the spectrum – whose chromaticity points lie outside the chromaticity diagram, an expert of colorimetry would correct them: ‘this is not possible’.

If we formulate a question to *artificial intelligence* targeting the same thing, we get the result delivered in Fig 1.

Is it possible that the chromaticity point of a real light source lies outside the CIE xy chromaticity diagram?

No, the chromaticity of a real light source cannot lie outside the CIE xy chromaticity diagram.

Here’s why:

1. **CIE xy Diagram Boundaries:** The CIE 1931 xy chromaticity diagram encompasses all possible chromaticity values for visible light. It is a projection of the 3D color space onto a 2D plane, with the boundary curve representing monochromatic (pure) colors at different wavelengths.
2. **Real Light Sources:** Any real light sources will have a chromaticity point that corresponds to a mixture of wavelengths within the visible spectrum, even if the source is monochromatic or combines several wavelengths. Therefore, its chromaticity point must fall within the boundaries of the xy diagram, which represents the full range of visible color perception.

Figure 1 – Question posed to artificial intelligence and the response (ChatGPT 3.5, 6 NOV 2024)

In the well-respected reference book of Hunt and Pointer (Hunt, 2011) we find the following statement: *The area within the spectrum locus and the purple boundary encloses the domain of all colours; this is because the spectrum locus consists of a continuously convex boundary so that all mixtures of wavelengths must lie inside it.*

In the *Encyclopedia of Color Science and Technology*, the chapter related to chromaticity coordinates contains the following statements (Westland, 2016): *The curved horseshoe-shaped locus of the chromaticity diagram is defined by the chromaticities of the monochromatic wavelengths of light. Since all real color stimuli are combinations of the monochromatic wavelengths, and given the earlier observation about how color mixtures are defined in the chromaticity diagram, it is clear that the gamut of all physically realizable colors is the convex hull constrained by the curved spectral locus.*

The convexity of the CIE 1931 chromaticity diagram (CIE, 1986a) has been just like an axiom – no chromaticity should be outside the boundary or with other words, outside the spectral locus. However, in this study, it is shown that it is possible.

2 First observations

For a special task at the firm the lead author of this study works for, simulations with LED spectra were performed. The LEDs used in a certain product (labelled as ‘amber’ LEDs here) were used as a reference to generate theoretical spectra (Fig 2) and a simple model function was applied that achieves good approximation, see Eq (1).

$$S(\lambda) = \exp_p \left(- \left| \frac{\lambda - c}{b} \right|^k \right) \quad (1)$$

where

$$\exp_p(x) = p^x.$$

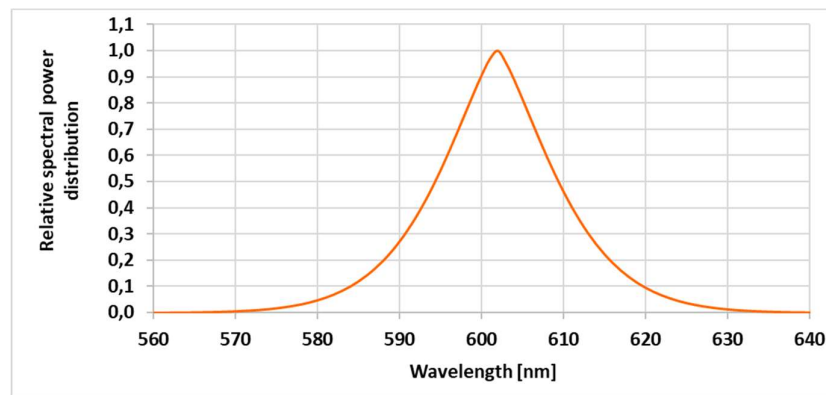


Figure 2 – A typical spectrum generated with the model function for amber LEDs

When random values were applied within a small range for the parameters of Eq (1); $p = 2,12 \pm 0,005$; $c = 601,88 \pm 0,02$; $b = 8,00 \pm 0,005$ and $k = 1,38 \pm 0,005$; the chromaticity points of the spectra generated with the model function appeared outside the CIE 1931 chromaticity diagram, see Fig 3.

Then, after some manual trials, a spectrum consisting of only two monochromatic lines, defined by Eq (2), showed similar behaviour, see Fig 3.

$$S(589 \text{ nm}) = 1,00 \quad S(611 \text{ nm}) = 1,67 \quad S(\lambda) = 0 \quad \text{elsewhere} \quad (2)$$

Chromaticity points of regular spectra falling outside the CIE 1931 chromaticity diagram were surprising, so three experts, all of them having a PhD degree related to colorimetry, verified the calculations. No errors were found.

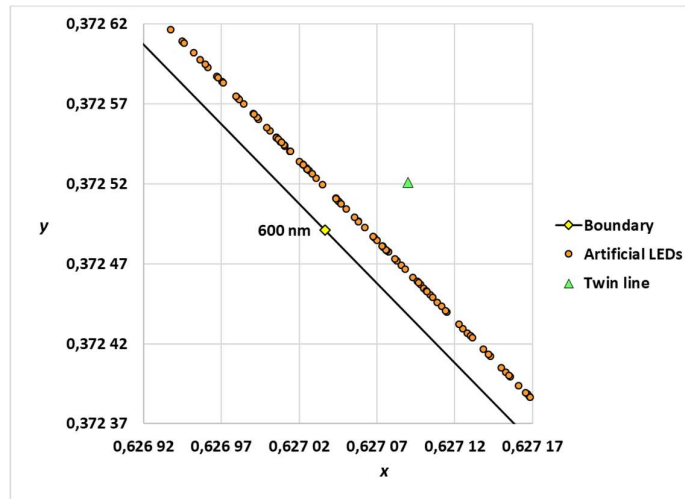


Figure 3 – Chromaticity points of ~100 random spectra, outside the CIE 1931 chromaticity diagram (orange dots), of the monochromatic spectrum line at 600 nm (yellow diamond) and of the spectrum of only two lines (green triangle)

3 Analysis

If somebody wants to study the boundary of the CIE 1931 chromaticity diagram in the spectral range where the monochromatic colours are called orange or amber, some magnification would be necessary. Despite the fact that this part of the spectral locus approximates a straight line, the problem with magnification is that this line is neither horizontal, nor vertical. However, the chromaticity diagram can be rotated around the origin without shape distortion. Thus, as the subsequent step, the diagram was rotated based on Eq (3).

$$\begin{bmatrix} x_\alpha \\ y_\alpha \end{bmatrix} = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix} \times \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} x_{ofs} \\ y_{ofs} \end{bmatrix} \tag{3}$$

In practice parameters $\alpha = 44,88^\circ$; $x_{ofs} = 0,6$ and $y_{ofs} = 0$ were applied. Note that x_{ofs} is only used to locate the entire diagram in the first quarter. The result is shown in Fig 4.

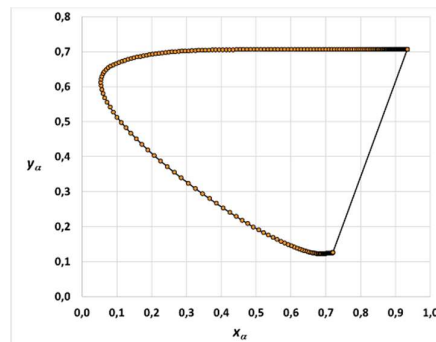


Figure 4 – The CIE 1931 chromaticity diagram rotated by $\alpha = 44,88^\circ$ and shifted by $x_{ofs} = 0,6$ ($y_{ofs} = 0$) – the dataset was taken from the CIE standard (CIE 1986a)

With the diagram in Fig 4, it is already possible to apply strong magnification in the vertical direction and to study the spectral locus on a wider range. The result is demonstrated in Fig 5.

The shape of the spectral locus starting at 572 nm clearly shows that in this range the convexity of the diagram is violated, in some ranges strongly violated. This figure proves the postulation that the chromaticity point of some real spectra can fall outside the diagram.

After the results introduced above it is apparent why the chromaticity of that simple two-line spectrum defined by Eq (2) is located outside the diagram. When the additive mixture of two monochromatic colour stimuli is taken, the chromaticity of the mixture is still on the line connecting the two original monochromatic chromaticity points, see Fig 6.

The authors of this paper chased real LEDs whose chromaticity points were outside the diagram. The trials were crowned with success. There exist real, not only simulated LEDs, whose measured spectra ensure that their chromaticity points are outside the diagram.

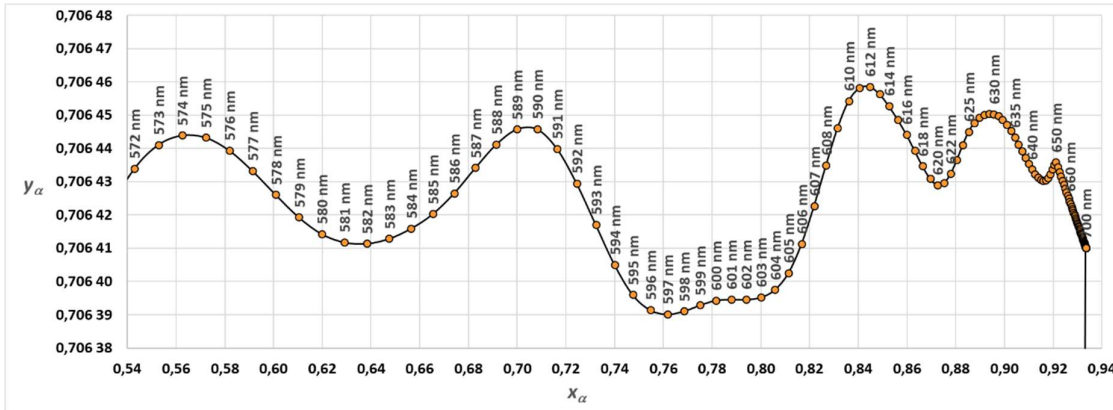


Figure 5 – The CIE 1931 chromaticity diagram rotated by $\alpha = 44, 88^\circ$ and shifted by $x_{ofs} = 0, 6$ ($y_{ofs} = 0$). Strong magnification applied

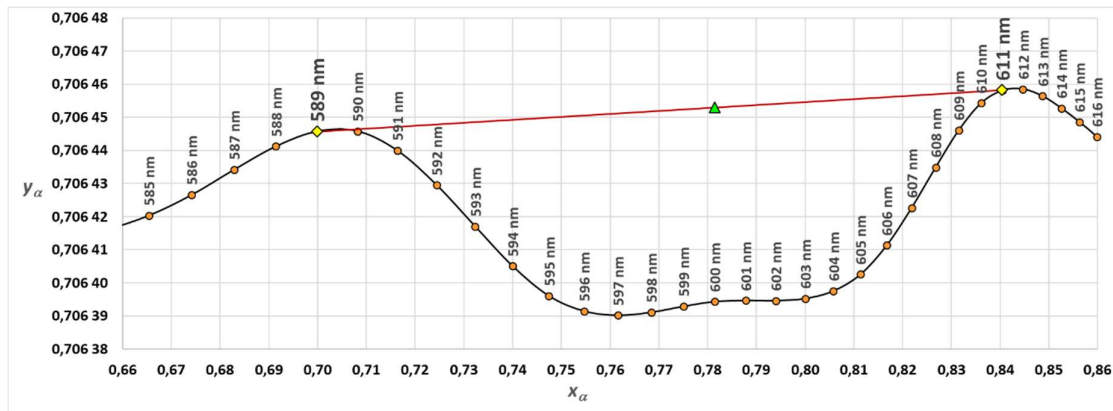


Figure 6 – Additive mixture of two monochromatic colour stimuli (589 nm and 611 nm). As the CIE 1931 chromaticity diagram is not convex in this spectral range, the chromaticity of the mixture lies outside the diagram

4 Signed curvature

At this stage of the study a useful tool shall be found with which the convexity of the chromaticity diagram can be expressed. The mathematical discipline differential geometry offers the concept of signed curvature of plane curves for this purpose (Woodward, 2019).

Let $x \in \Lambda \rightarrow \mathbb{R}$ and $y \in \Lambda \rightarrow \mathbb{R}$ be two functions for which $\Lambda \subset \mathbb{R}$. Set Λ refers to the wavelength range, while \mathbb{R} is the set of real numbers. Then, point set $(x(\lambda), y(\lambda)) \in \mathbb{R}^2, \lambda \in \Lambda$, forms a regular plane curve and this definition specifies a parametric plane curve. The signed curvature of the plane curve can be calculated as

$$k(\lambda) = \frac{x'(\lambda) \cdot y''(\lambda) - y'(\lambda) \cdot x''(\lambda)}{(v(\lambda))^3} \tag{4}$$

where

$$v(\lambda) = \sqrt{(x'(\lambda))^2 + (y'(\lambda))^2} \tag{5}$$

For computing the values of functions x' , y' , x'' and y'' central finite differences of the 4th order were used. The formulae are as follows. The step size (usually denoted by h) was chosen to be unity. Symbol i means the i^{th} wavelength value in set {382 nm, 383 nm, ..., 777 nm, 778 nm}.

$$Df(\lambda_i) = \frac{f(\lambda_{i-2}) - 8f(\lambda_{i-1}) + 8f(\lambda_{i+1}) - f(\lambda_{i+2})}{12} \tag{6}$$

$$D^2f(\lambda_i) = \frac{-f(\lambda_{i-2}) + 16f(\lambda_{i-1}) - 30f(\lambda_i) + 16f(\lambda_{i+1}) - f(\lambda_{i+2})}{12} \tag{7}$$

The sign of curvature k as a function of the wavelength is plotted in Fig 7. (Note that this is not the signed curvature plot, only the sign of the curvature.)

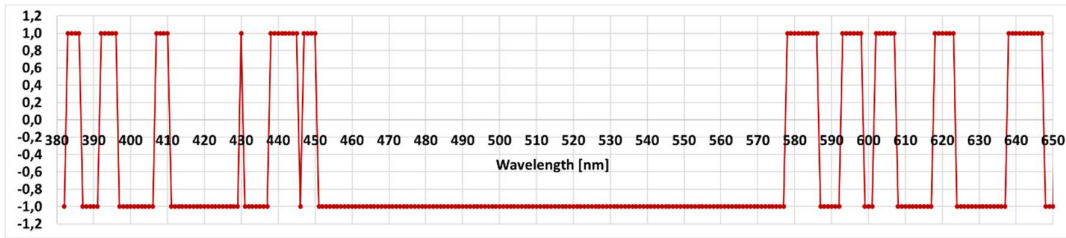


Figure 7 – Sign of the curvature of the spectral locus in the CIE 1931 chromaticity diagram as a function of the wavelength

First let us investigate the function in Fig 7 between 570 nm and 650 nm. There are five small ranges where the sign of the curvature is +1. If we set these five wavelength ranges against the labels of the spectral locus in Fig 5, it can be stated that they are subsets of the wavelength ranges where the chromaticity diagram is not convex. This proves that the function of the signed curvature can be a useful tool to find other problematic locations.

Based on the sign of the curvature function, the spectral locus was investigated in wavelength ranges [380 nm, 413 nm] and [428 nm, 453 nm]. Related to these two intervals the chromaticity diagram was rotated again, see Fig 8.

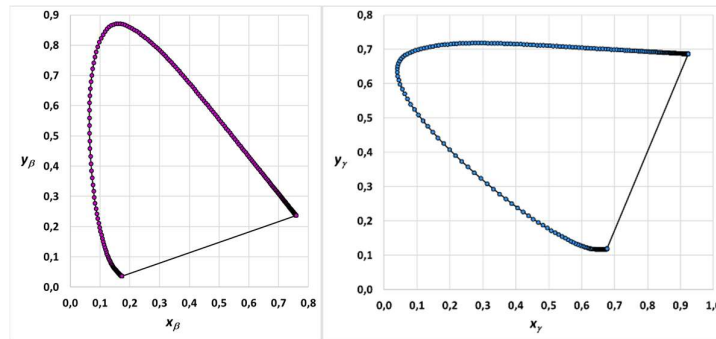


Figure 8 – The CIE 1931 chromaticity diagram rotated by $\beta = -6^\circ$ and shifted by $y_{ofs} = 0,05$ ($x_{ofs} = 0$) for studying the spectral locus in wavelength range [380 nm, 413 nm], then by $\gamma = 41,6^\circ$ and shifted by $x_{ofs} = 0,55$ ($y_{ofs} = 0$) for range [428 nm, 453 nm]

The spectral locus in the chromaticity diagram can be seen in Fig 9 and Fig 10 for the two ranges respectively. Note that also here strong magnification is applied along the vertical axis. Studying Fig 9 and Fig 10 it can be observed that the chromaticity diagram is not convex in the spectral ranges just as forecasted by the signed curvature function.

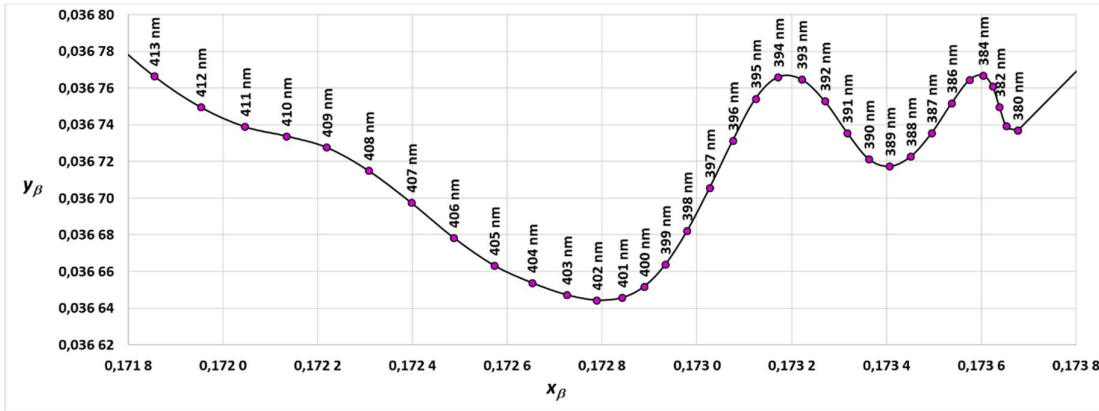


Figure 9 – The CIE 1931 chromaticity diagram in the range [380 nm, 413 nm] rotated by $\beta = -6^\circ$ and shifted by $y_{ofs} = 0,05$ ($x_{ofs} = 0$). Strong magnification applied

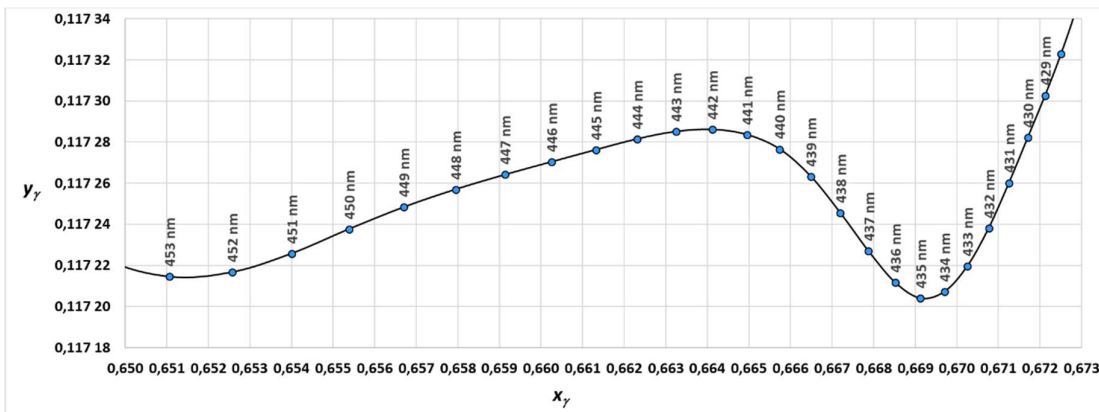


Figure 10 – The CIE 1931 chromaticity diagram in the range [428 nm, 453 nm] rotated by $\gamma = 41,6^\circ$ and shifted by $x_{ofs} = 0,55$ ($y_{ofs} = 0$). Strong magnification applied

5 The curvature at the longer wavelength range

Let us investigate the sign of the curvature function at the longer wavelengths, in the range already investigated ($\lambda > 650$ nm), up to 700 nm. The values fluctuate frequently between -1 and $+1$, see Fig 11. However, if not only the sign but the signed curvature itself is plotted, the values of the function above 652 nm vanish, i.e. they tend to be very close to zero, see Fig 12. This fact suggests that the violation of convexity may be neglected – if present at all. The spectral locus in the rotated diagram is plotted in Fig 13. It can be stated that in this spectral range, i.e. approximately from 650 nm to 700 nm, one does not need to be concerned about the convexity of the diagram. Only negligible deviations from a straight line appear in this range.

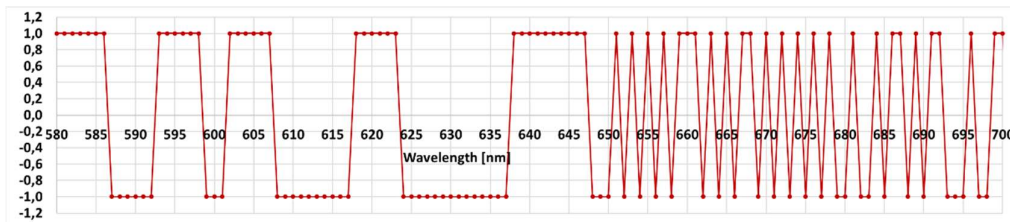


Figure 11 – Sign of the curvature of the spectral locus in the CIE 1931 chromaticity diagram as a function of the wavelength

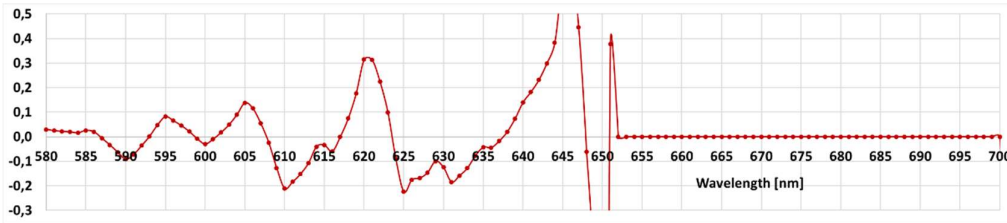


Figure 12 – The curvature of the spectral locus in the CIE 1931 chromaticity diagram as a function of the wavelength

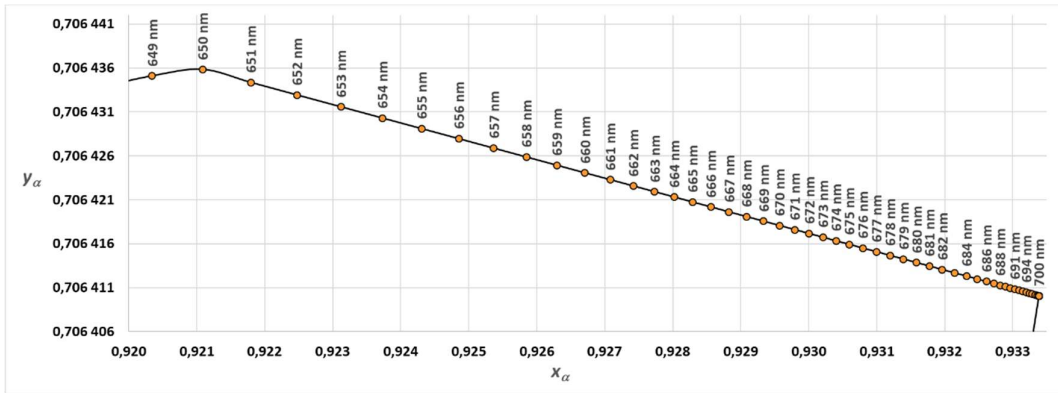


Figure 13 – The spectral locus of the CIE 1931 chromaticity diagram at longer wavelengths ($\lambda > 650$ nm). $\alpha = 44, 88^\circ$; $x_{ofs} = 0, 6$; $y_{ofs} = 0$

6 The boundary beyond 698 nm

Let us investigate the sign of the curvature function beyond 698 nm. Again, the values fluctuate frequently between -1 and $+1$, see Fig 14. But if the values of the curvature function itself are studied, it can be observed that something strange happens here, see Fig 15. These values are bigger by several orders of magnitude than those plotted in Fig 12.

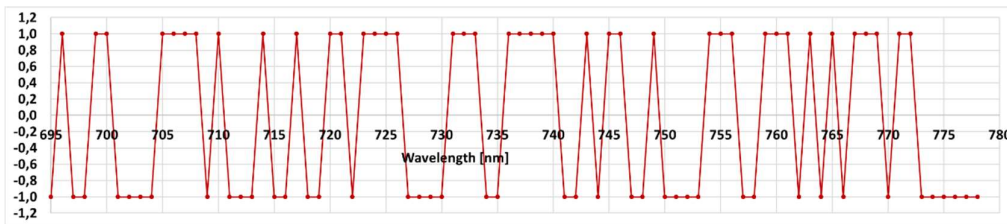


Figure 14 – Sign of the curvature of the spectral locus in the CIE 1931 chromaticity diagram as a function of the wavelength ($\lambda > 695$ nm)

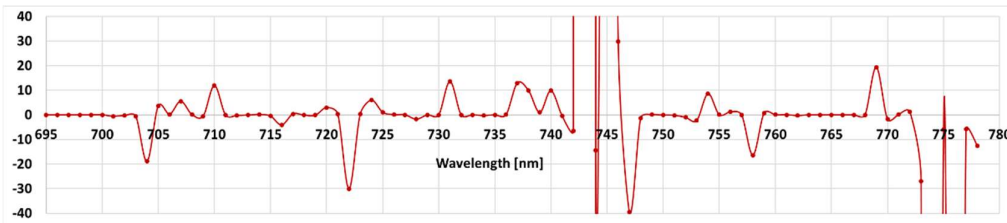


Figure 15 – The curvature of the spectral locus in the CIE 1931 chromaticity diagram as a function of the wavelength ($\lambda > 695$ nm)

In Fig 13, the last label shown is 700 nm. With this resolution and diagram style, all chromaticity markers belonging to higher wavelength values overlap. Thus, at the very end of the visible

spectral range it carries little meaning to talk about convexity or non-convexity. However, a very strange phenomenon can be recognized here. The directionality of the spectral locus turns backwards and then forwards again several times. The frequent change of the directionality is another interpretation of the vibrating sign of the curvature function.

Fig 16 contains two graphs. Labels are added in such a manner that the displayed ones do not occlude one other. Even the upper graph shows that the spectral locus loses the one-way directionality. The chromaticity points belonging to increasing wavelength values are not in an ascending order. The increasing monotony is violated several times. The magnification at the lower graph is so strong that this scaling clearly shows that the spectral locus is not a real boundary. Studying the lower graph one may conclude that at the extension of the colour matching functions beyond 700 nm this property had not been fully recognized. Consequently, there is a branch that should not be there.

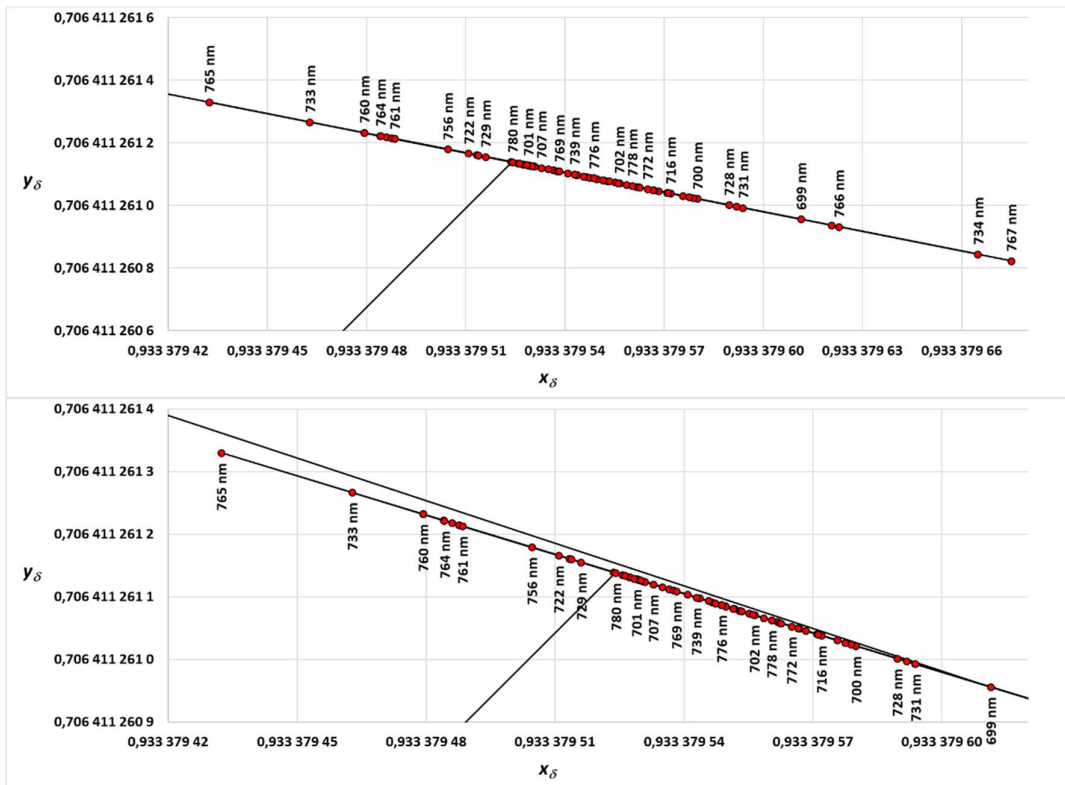


Figure 16 – The spectral locus beyond 689 nm. Rotation parameters: $\delta = 44,880 2^\circ$; $x_{ofs} = 0,6$ and $y_{ofs} = 0$. Very strong magnification applied

7 The CIE 1964 chromaticity diagram

In the previous chapters, it has been proven that the CIE 1931 chromaticity diagram is not convex. Now let us investigate the CIE 1964 chromaticity diagram (CIE, 1986a).

The signed curvature function can be studied in Fig 17. Beyond 450 nm the values are very near to zero. The graph suggests that if there are spectral ranges in which the convexity of the diagram is violated, they must be below 415 nm.

Applying appropriate rotations and magnification, the problematic areas can be found, see Fig 18. This means that also in the case of the CIE 1964 chromaticity diagram the convexity is violated.

The phenomenon at the longer end of the visible spectral range that was demonstrated with Fig 16 is much worse here. It can be seen even with the naked eye that the original diagram (no rotation applied) has a small 'tail' there, highlighted within the blue square in Fig 19.

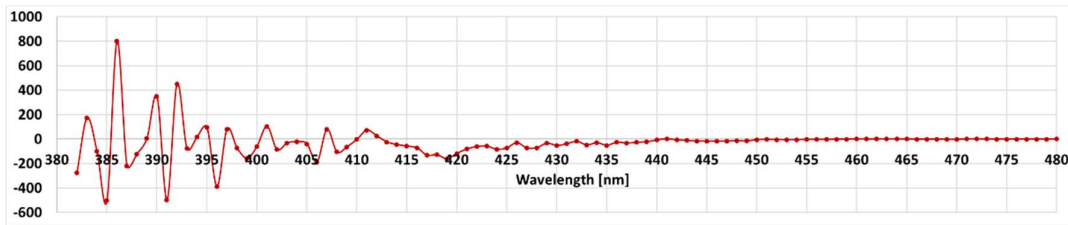


Figure 17 – The curvature of the spectral locus in the CIE 1964 chromaticity diagram as a function of the wavelength

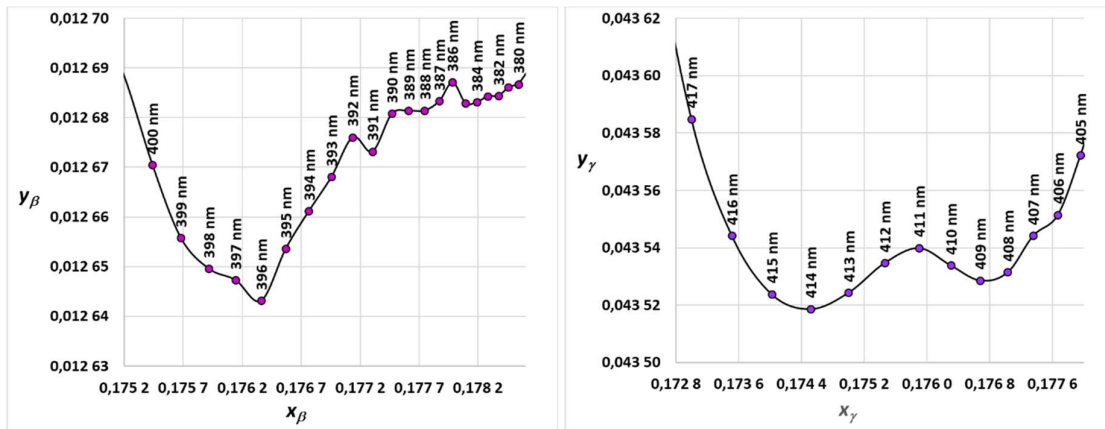


Figure 18 – The CIE 1964 chromaticity diagram in the range [380 nm, 400 nm] rotated by $\beta = -18^\circ$ (left) and in the range [405 nm, 417 nm] by $\gamma = -8^\circ$ (right). In both cases shifted by $x_{ofs} = 0$ and $y_{ofs} = 0,05$. Strong magnification applied

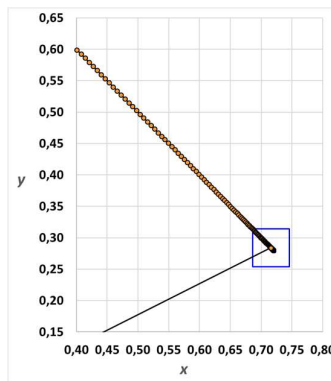


Figure 19 – The CIE 1964 chromaticity diagram has a small ‘tail’ at the longer end of the visible spectral range – marked with the blue square

On the ‘tail’ of the CIE 1964 chromaticity diagram the monochromatic chromaticity points follow the same direction till 700 nm. Then they stop and reverse, see Fig 20. The turning point is 700 nm. This means that when monochromatic colour stimuli of a wavelength between 657 nm and 779 nm are mixed with colour stimuli of a wavelength close to 380 nm, the chromaticity of the mixture will be outside the diagram, on the outer side of the purple line. Beside the non-convex parts of the diagram it represents another possibility to have chromaticity points of real spectra outside the diagram.

The colour matching functions related to the cone fundamentals are out of the scope of this paper, hence they are only published in a tabular form with a step size of 5 nm (CIE, 2006). However, it can easily be demonstrated that the fundamental chromaticity diagram is not convex in the range of [390 nm, 405 nm]. It also has a ‘tail’ and the behaviour of the chromaticity points beyond 700 nm is very similar to that described in the CIE 1964 colour system.

