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”Like stars are moving in the sky” – life of an infrared photographic studio

Don’t be hasty.
Though by your labour others profit,
merely working precisely and fine
just like stars are moving in the sky
is but worth it.

Attila József
(1905-1937)

Keywords: infrared spectroscopy, multivariate data analysis, imaging

1. SUMMARY

Today, users can choose from many options according to their goals when they turn to the toolbox of vibrational spectroscopy when answering their questions. This diversity is reflected in the structure, sample handling, and measurement technology of the devices. It is enough to think of handheld devices that enable on-site measurements in incoming raw material warehouses, or bench-top devices for quality control laboratories, or in-/on-line devices for production technologies. In addition, chemical imaging (CI) techniques have also gained ground. Mathematical, statistical, and chemometric methods are breathing life into the army of infrared spectra provided by the hardware, which are capable of extracting the information inherent in large data sets (big data). In the article, the development and embedding of infrared techniques from academic research to agricultural and industrial applications can be traced by highlighting examples of the last 25 years – but not only through spectroscopic tools, but also through people.

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2. Introduction

As a young adult, the Győr ”Festival of Photographers” **[1]** left me with many, many good memories. The medium consisted of lights and sounds, i.e., waves, it evoked a feeling and opened a window to new, unknown worlds, giving me a better understanding of it. In our small research group, we are striving to do the same: with the help of the infrared range of electromagnetic radiation we seek to understand the chemical (and often physical **[6, 7, 8]**) history of the substance under study through the interaction of waves with the matter investigated, as so many have done **[4, 5]** since Sir William Herschel **[2, 3]**.

2.1. Characteristic NIR absorption bands

Almost all functional groups needed to study a biological system provide signals in the range closer to red, also called near infrared (NIR), of non-destructive molecular (or vibrational) spectroscopy, which requires little or no sample preparation (***Figure 1***). Life-giving water provides signals through its O–H groups; structural or reserve proteins through the C=O and N–H groups of the peptide bonds between amino acids and through their side chains; lipids through their saturated (C–C) or unsaturated (C=C) carbon-carbon bonds, and through the C–H vibrations of their large numbers of methyl (–CH_3) and methylene (–CH_2–) groups, absorbing the photons with wavelengths characteristic of them, and thus moving to higher energy levels. Carbohydrates, as polyhydroxy-oxo compounds, are a bit like mules: the vibrations of the groups listed above (O–H, C=O, C–H) appear together.

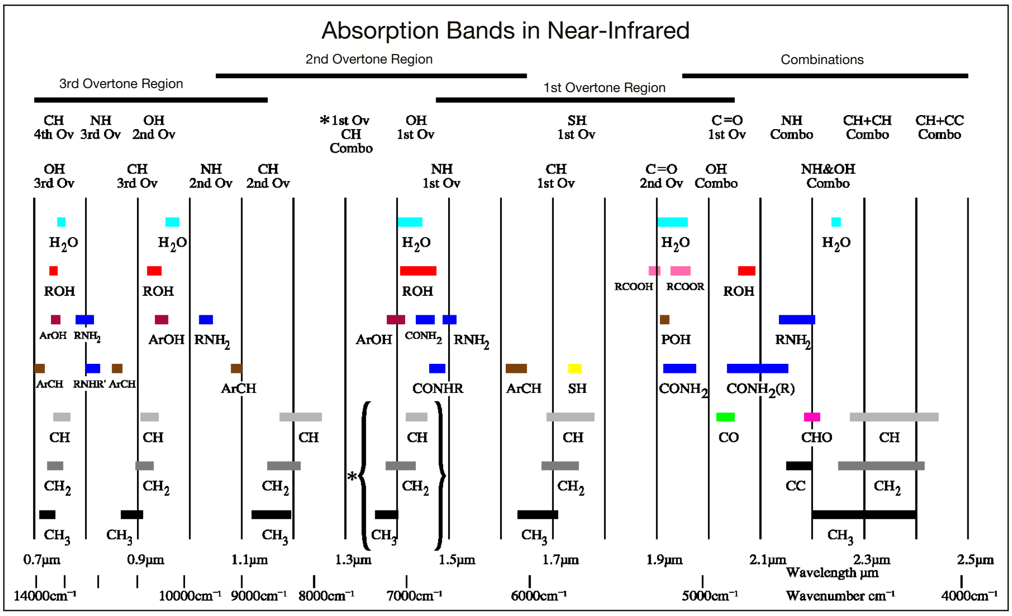

Figure 1. Group absorptions in the near-infrared range ***[6]***

2.2. Multi variate data analysis in the NIR technology

And this brings us to the second so-called field of our interdisciplinary science after (N)IR spectroscopy, multivariate (data) analysis (MV(D)A), the magical world of chemometrics and statistics (i.e., mathematics as a common denominator), which we are constantly learning from Professors Sándor Kemény and Károly Héberger (professors at the Budapest University of Technology and Economy. The Ed.), still amazed by their knowledge, experience and pedagogical sense **[9, 10]**. In our area, the need for these sciences stems from two main sources.

Firstly, the macro-components listed above (together with the micro-components) make up the whole, the living. Given the profile of our department, it is mainly these complex (plant, animal, human) systems that are studied “*as is*” or in a processed form (crops, foods, tissues), always resulting in complex, envelope-like spectra. The analysis of these (e.g., identification or assignment of spectral peaks) is inconceivable without smoothing with moving averages, derivative-sensitized peak resolutions or baseline shifts eliminated by normalization. From another professional topic, an example is the case number diagram for the SARS-CoV-2 pandemic, where the change in the epidemic data provided a good indication of the current epidemic situation by plotting the moving averages (***Figure 2***).

Secondly, spectrum-based identification or the construction of qualitative or quantitative models also requires mathematical tools: sometimes only a single correlation calculation is needed, sometimes more serious vector algebra or operations with matrices.

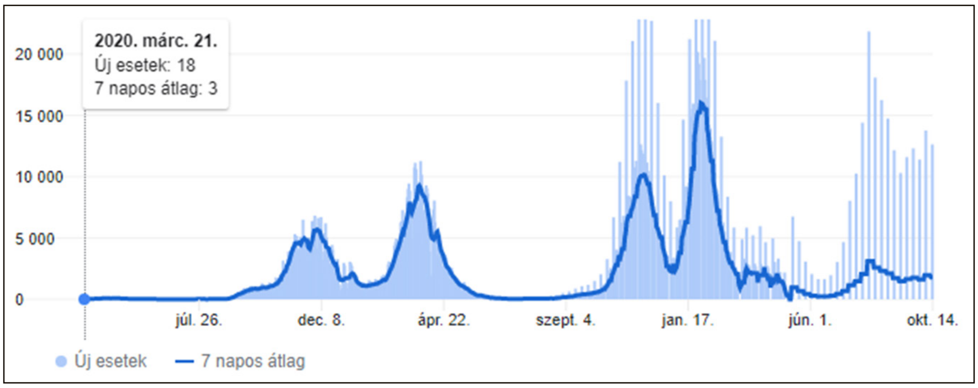

Figure 2. New COVID-19 cases – data received (as columns) and the 7-day moving average (as a bold line) ***[11, 12]***

It may be clear from the above that living in the age of Industry 4.0 (***Figure 3***) and circular economy **[13]**, whether it is precision agriculture, the food industry using knowledge-based technologies, or the pharmaceutical industry with its PAT and QbD approach, non-destructive spectroscopic sensors (NDSS) are coming to the fore as the main tools, be it fiber-optic sensors in tubes (***Figure 4***) or cameras mounted on conveyor belts measuring in the UV/Vis/NIR range.

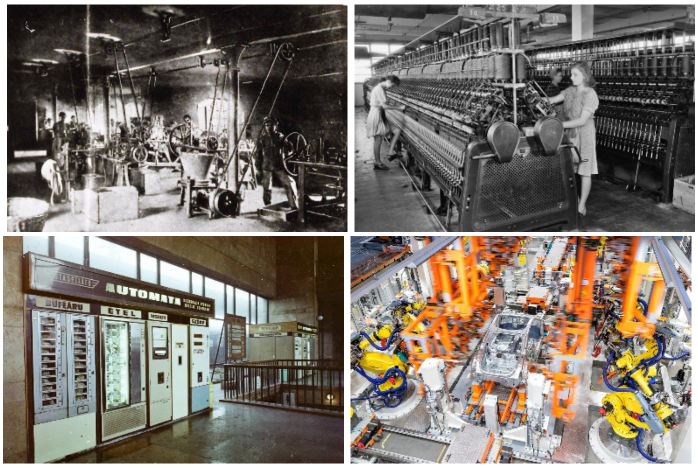

Figure 3. Győr vs. Industry 1.0: match factory, 2.0: flax weaving mill, 3.0: food and drink vending machine, 4.0: car factory ***[14, 15, 16, 17]***

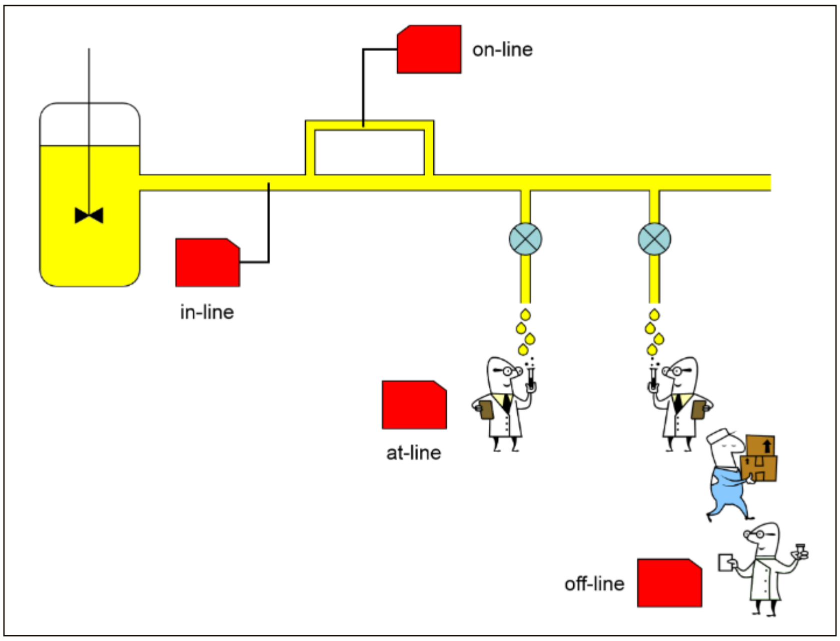

Figure 4. Relationship between sampling and measurement locations ***[18]***

3. The application of infrared technics at the Department

The transition from foods to drugs (either this way or that) is a recurring theme in our work, especially if we look back at our career over the decades since the 1990s. For example, the experience gained in the measurement of wines, sparkling wines, liqueurs, spirits **[19]**, beers and palinkas **[20]** has been useful in the development of techniques for real-time monitoring of the fermentation processes of monoclonal antibodies **[21, 22]**. If we had been working at product manufacture, i.e., *upstream*, we had to help in purification, i.e., *downstream*, if we were able, for example in the qualification of column packings used in preparative chromatography **[23]**. In all cases, the goal is, as in the eternal struggle of the world (living inside us), to recognize the difference between good and bad (based on experience = data (*data-driven*)), to find the cause of being bad (error analysis), to eliminate it and put it on the right track (*golden batch*). But perhaps the smartest thing to do, in the spirit of “better safe than sorry”, is to take preventive action (*predictive maintenance*) based on the warning signs before bad things happen. Even the latter can be very helpful, when the focus is not necessarily on the accuracy and precision of the specific metric, but on its variability, dynamics and trend.

It can be mistaken to think that on-site (*in situ*), immediate (*just-in-time*) measurements are only the prerogative of producers of high value-added biotech products. Agricultural sensors can form the same kind of network as IoT (*internet of things*) devices in a smart home. The added value is smaller: but the material flows can be orders of magnitude higher and, as we know, look after the cents and the euros will look after themselves. Whether it’s a feed mixer with a batch approach, working with dedicated recipes **[24]** or a continuous bioethanol plant with a constant quality goal, there are NIR instruments containing no moving optical elements (thus unaffected by vibrations and shocks). Both of these examples are based on corn and/or wheat, which is not surprising given the development of NIR spectroscopy. These are the basic food materials the investigation of which pioneered the diffuse reflectance NIR analysis of solid materials by Karl Norris of the USA and Phill Williams of Canada in the 1960s and 1970s **[5]**. Looking a little further, it is perhaps worth quoting Harari’s thoughts here, citing the foreword of Péter Hahner: “[...] it was not man who domesticated wheat, but rather wheat domesticated man, since *homo sapiens* has been living in houses since he switched to cereal production” **[25]**.

Wheat plays an important role not only in the life of mankind, but also in the life of our group at the Department: the first NIR spectrometers were obtained mainly to measure wheat, thanks to János Varga and later András Salgó **[26, 27]**, and the Cereal Group of Sándor Tömösközi provided us with constant ammunition in the field of cereal research **[28, 29]**. During the maturation dynamics of wheat, changes of the main components (moisture, proteins, carbohydrates) were followed over time by NIR spectroscopy **[30, 31, 32]**, then by capillary electrophoresis with the help of our colleague Éva Scholz, then by liquid chromatography **[33]**.

The life of a plant seed often continues in the mill, losing its compactness, its integrity, being broken into elemental pieces, and being reborn in different forms. Chaff is separated from wheat, the husk and germ from the kernel, meal from flour, these are the grinds fractions used for our daily bread, or for the formation of our reserves (***Figure 5***).

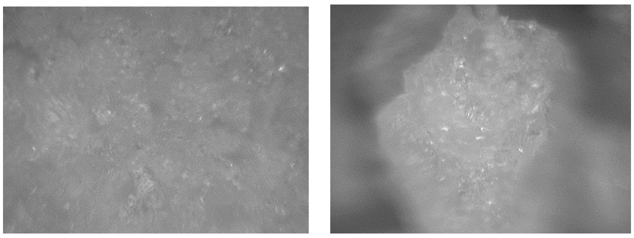

Figure 5. Microscopic images (400×500 µm) of wheat flour (BL 55) and pasta industry wheat flour (TL 50) ***[34]***

The need came from plant breeders to replace the grinding of 200 g of wheat grain for classical wet chemistry analyses with the processing of 10 g of material. In the initial stages, only a few spikes of grain are available, so analytical possibilities are severely limited. This led, thanks to domestic developments **[35]**, to the birth of a micro-mill, the milling properties of which were compared by means of the NIR spectra of the milling fractions with that laboratory mill, which is able to grind 200 g of seed, **[36]**. After two decades, we are still interested in similar questions: how grinding and milling affects NIR spectra through light scattering due to mesh size, which can be used to profile different laboratory grinders, helping the decision of users when switching to a different model **[8]**, or how to monitor a large-scale milling process, following pasta flour yields **[37]**, or the heat treatment of the resulting fractions **[38]**.

To the frequently arising question “What’s in the sample?”, NIR photons, still non-destructive but already with the energy needed for proper penetration, have helped many times, whether for investigations through packaging materials, or for looking into smaller or larger green samples (watermelon, algae). The former is necessary because, in many places, people work with substances that are hazardous to health and must be removed from the packaging material before use in order to identify and qualify them. For this reason, model systems have been developed where the extent of absorption of plastics can be detected, and their impact can be reduced by variable selection and/or mathematical treatments **[39]**. Of course, we also help our colleagues where we can, in our area of expertise. Pál Maák (BME TTK, Institute of Physics, Department of Atomic Physics) and his colleagues have built a prototype (***Figure 6***) that uses NIR lasers to measure the sugar content of watermelons – an order of magnitude leap in measurement sensitivity compared to the apple, kiwi and orange analysis methods of foreign researchers. Here, we provided support in measuring the sugar absorption peaks, the wavelength – indirectly the choice of lasers. Here, we have provided support in measuring the “sugar peaks” and selecting the wavelengths and thus, indirectly, the lasers **[40]**. To Áron Németh (BME VBK ABÉT, Laboratory of Fermentation Experiments) and his colleagues we were able to offer a solution in the mid-infrared (i.e., analytical) range for the selection of algal species and product yields (i.e., specific lipid amounts as sources of biodiesel) under small-scale cultivation conditions **[41]**. We strive to maintain integration not only at the level of research groups within the department and the university, but also with national and international universities and research institutes through our professional and grant activities, seeking new applications for the spectroscopic techniques we use **[42]**.

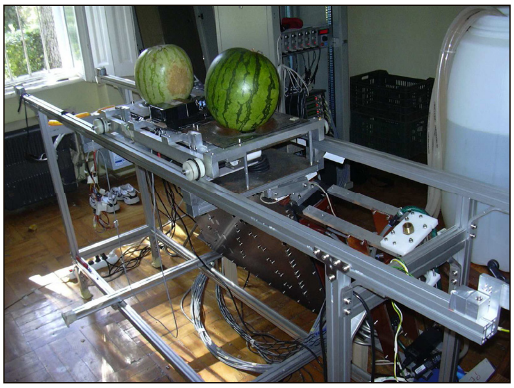

*Figure 6. Prototype for measuring the sugar content of watermelons based on NIR technology **[43]***

Integration can be achieved not only between people but also between data sets. Just as we demonstrated in 2006 and 2006 how to combine optical NIR spectra and rheological viscosity curves **[44, 45]**, we are working on new solutions for data fusion 15 years later with Pál Péter Hanzelik, representing large-scale industrial background (MOL Nyrt. – Hungarian gas and oil company. The Ed.) with coordination and active participation **[46]** and Zsombor Kristóf Nagy, who enables connection within the BME-FIEK framework and also involves our research group in the work of the Pharmatech Pharmaceutical Technology Laboratory. Similarly, a fruitful collaboration, now going back to several years, has been established with Márton Bredács, a pillar of the Polymer Competence Center Leoben (PCCL) which works closely with the University of Leoben, in the multisensory selection and classification of plastic wastes using several spectroscopic sensors (Vis, NIR, Raman) **[47]**.

A significant milestone in the life of the group of our Department was the advent of imaging technology. From the early 2000s, presentations and exhibitors at international conferences and publications proliferating in the field showed that “commercialization” (i.e., mass production and wider marketing after prototypes and limited series) had begun. Sticking to what we had been doing, we investigated plant seeds **[48]**, but in addition, a more classical human line was also initiated by the persistent work of Endre Kontsek and Adrián Pesti (our former students, now at the Institute of Pathology, Forensic and Insurance Medicine of Semmelweis University). After studying kidney and gallstones **[49]**, as suggested by our doctors, we turned our attention to soft tissues, tumors and cancerous cell lines **[50, 51]**, hoping to contribute to the development of digital pathology or, as a long-term goal, to the development of real-time tumor identification during surgery. We owe a lot to Alfréd Kállay-Menyhárd and his colleagues (in chronological order, Péter Müller, Dóra Tátraaljai, József Hári and Balázs Kirschweng) from a co-institute (BME VBK FKAT Plastics and Rubber Laboratory), the assignments from whom have contributed to our research on plastics microscopy, be it biodegradable polylactic acid/thermoplastic starch (PLA-TPS) mixtures (***Figure 7***) or the failure analysis or reverse engineering of various products (adhesives, foils, medical instruments, electric engine coatings).

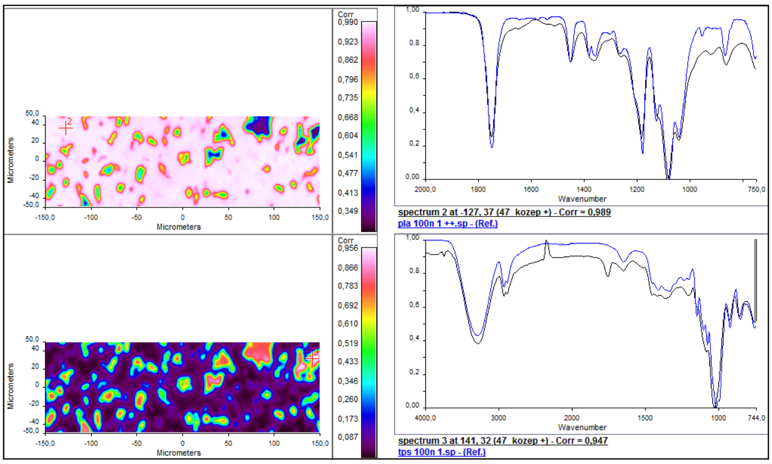

Figure 7. Distribution analysis of a polylactic acid/thermoplastic starch (PLA-TPS) mixture on IR-imaging based correlation maps (left) using the spectra of reference materials (right, in blue; top: PLA, bottom: TPS) ***[52]***

And speaking of failure analysis, Péter Gordon and his enthusiastic team (BME VIK ETT EFI-labs) are a factor in this area who cannot be ignored, their sample preparations and documentations greatly assist not only our imaging tasks listed above, but also, for example, the cross-sectional analysis of laminated packaging materials (***Figure 8***).

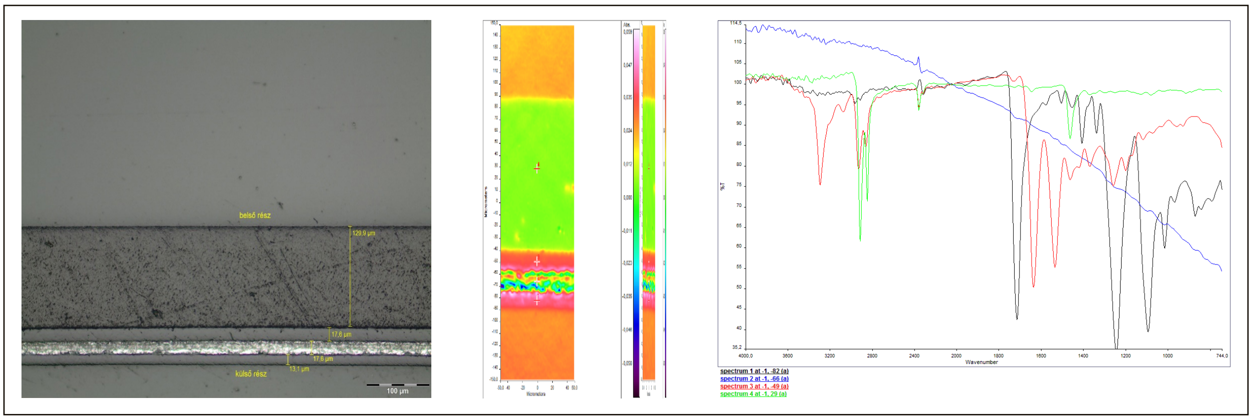

Figure 8. Cross-sectional view of a multilayer food packaging material (bag of chips, left) ***[53]****, in IR microscope (middle), and IR spectra of the selected points in each layer* ***[54]***

Still on the subject of plastics, in terms of their environmental aspects, it is microplastics that we are most confronted with these days in everyday and scientific news media. Microplastics (and the chemicals they bind) that enter the food chain through contamination of the inanimate environment can also be harmful to health. In collaboration with Gábor Bordós and his colleagues (WESSLING Hungary Kft.), we have developed a methodology for the application of the infrared range to monitor different types of our waters **[55, 56]**.

As in the previous example, we always come back to man. And once the disease is found, in Western medicine, the next step is the medicine, the pill, and like all good things, these are counterfeited as well. With József Horgos (WESSLING Hungary Kft.) we started to map out this area (literally) **[57, 58]**, and later on we received support from Szilvia Lohner (OGYÉI) in the form of test substances. However, not only counterfeiting, but also (non)compliances of technological origin and the model systems built for formulation development can also be investigated in terms of the presence and distribution of ingredients. The aim is to have a machine vision that classifies not only in the UV and Vis, but also in the NIR range, estimating drug release based on models **[59, 60]**.

One of the most beautiful challenges in terms forecasting is predicting earthquakes. If we recall the earthquake of June 28, 1763, which shook Komárom, Győr and Zsámbék, with a magnitude of 6.3 and claiming 63 lives, and which led to the order to circle the herma of St. László in the city of Győr to avoid further earthquakes (***Figure 9***), the context becomes clear **[61]**. I consider the collaboration with István János Kovács and his colleagues, who are members of the Research Institute of Earth and Space Physics at ELKH and the Lithospheric Fluid Research Laboratory at ELTE TTK, a godsend.

Solids and liquids in mixtures, solutions or even colloidal form, often organized into living systems, as complex biological systems are often measured, as could be seen in the examples so far, but gases ("mobile volatiles") have been left out so far. We cannot take the credit for the measurements this time either. Our geologist colleagues have created that so-called Lithospheric Physics Unit (the first integrated geodynamic station in Central Europe) **[62]**, enabling the very exciting time-series analysis of the measured IR spectra (and other data). However, we should not forget the question to be answered: what can be seen on the changes in soil CO_2 levels, which as a fluid also exhibits tidal movements, and may suddenly become more pronounced due to tectonic movements. Could this be a harbinger of earth movements that are being triggered by the collision of African and European plates? Parts of the big puzzle are the fluids trapped in rocks, which contain CO_2, water vapor and other gases, in the study of which we can help with our background in microscopy **[63]**.

Figure 9. A votive picture of Győr with the leaning towers to commemorate the earthquake (left) ***[64]*** *and the 1939 St. László day procession with the herma* ***[65]***

The picture of the work in our Department would not be complete without a few words about the research on linear and non-linear relationships. In real life: our nervous system, equipped with our sensory organs (as peripheral organs), helps us to survive the challenges of everyday life by learning non-linear solutions. In machine language: an artificial neural network (ANN) with multisensory sensors and machine learning (ML) with nonlinear solutions operates decision trees.

What would László Telegdy-Kováts László (Galgóc, December 5, 1902 – † Budapest, May 11, 1987, chemical engineer, college professor) (***Figure 10***) say, who is remembered by CSEMADOK as follows: "He matriculated from the high school of Nyitra in 1919. Obtained his engineer's diploma from the Faculty of Chemical Engineering of the Technical University of Budapest in 1925. Became an assistant professor to Elek Sigmond (1873–1939), a chemical engineer and professor of agrogeology at the Technical University of Budapest, where he initially worked on soil biology. In the late 1920s, for an extended period he worked in England, where he became familiar with the modern methods of mathematical statistics and experimental design. In 1935, his interest turned to food chemistry, and as a researcher and a ministerial official, his main focus became the management and development of food technology. In 1950, he was appointed professor in the Department of Food Chemistry at the Faculty of Chemical Engineering of the Technical University of Budapest. He educated generations of engineers. His papers on the theoretical and practical issues of food quality are still relevant today. He is also credited with the development of novel food analytical methods. His attention also extended to food packaging technology. He considered the dissemination of scientific knowledge to be an important task and for many years he was president of the Society for Dissemination of Scientific Knowledge (TIT)" **[66].** We hope he nods in agreement **[67]**. In ***Figure 10***, we want to illustrate the technical possibilities in the field of optics that can be exploited through the application of artificial intelligence **[67]**.

Figure 10. Portrait of László Telegdy-Kováts in black and white (left) ***[68]****,* *and colored after machine learning (right)* ***[69]***

4. Conclusion and acknowledgement

Our research group's exploratory bioengineering nature combines the attributes of our specializations (applied biotechnology, health protection, food quality and environmental protection specializations), of which we were able to flash a picture of each within the framework of this article. We hope that we have created a good feeling by opening some window at a time while the movie continues...

* * *

First and foremost, I would like to thank András Salgó, the father of the NIR Spectroscopy Group: without him we would not be here either. Nor would we be here without those who, for many years, have entered the doors of K.II.3. or, more recently, of Ch 165 as PhD students and/or colleagues, namely (perhaps in chronological order) Gábor Sárossy, Réka Juhász, Tímea Gelencsér, Mária Hódsági, Eszter Izsó, Mónika Berceli, László Párta, Éva Szabó, Bence Kozma, Gabriella Besenyő and János Slezsák. Over the past 25 years, I have received a lot of strength, encouragement and examples, in addition to the members of the group, from Sándor Tömösközi, it was is understanding patience and trust in me that made it possible to take stock and this snapshot. I hope that the colleagues and students who have been part of our group think back on us as fondly as we think back on them, and we would like to thank the time spent working together, as we have also learned a lot.

I would like to thanks Sándor Nógrádi, and Géza Tóth (†), (Servitec Kft.) with whom we were able to experience the networking possibilities of NIR spectrometers, in addition to their agricultural and food applications, and gained insight into applications in the pharmaceutical industry, and to Miklós Lipták and Sándor Varju (PER-FORM Hungária Kft.) for broadening our vision and possibilities through access to analytical IR and microscopy techniques, thus opening the way to numerous collaborations with academic, research and industrial partners.

Dedicated to the memory of my Godfather

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