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Collaborative robots using computer vision applications in a chemical laboratory

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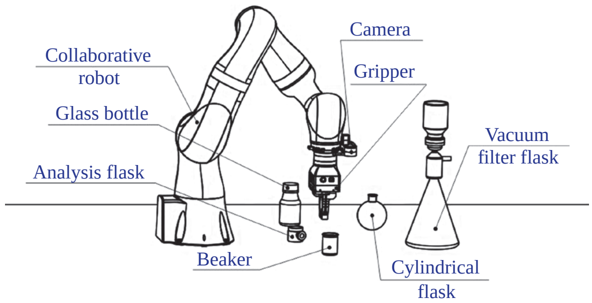
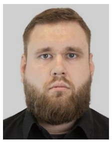
An overview of modern technologies in the field of laboratory automation, such as robotics and the use of computer vision, is presented. The main methods and equipment required for the automation process are discussed. A brief description of the implementation of collaborative robots and computer vision systems in automated laboratory work-stations is given, and a specific example of a centrifugation procedure is considered.



Keywords: computer vision, robotics, laboratory automation, cobots, High Throughput Screening, membrane, graphene oxide, polyethyleneimine, self-driving laboratories.

Introduction

Computer vision (CV) and robotics have found their uses in many applications nowadays. With the rapid growth of the technological level, the use of CV has expanded to several new areas, from smart city surveillance cameras that ensure safe infrastructure[1] to quality control in automated industrial plants.[2] CV mainly operates using neural network technologies that allow the recognition and identification of objects in the working



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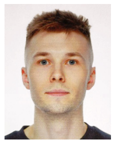

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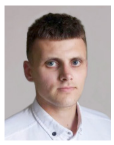

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field.[3,4] Solutions for the mentioned CV applications are actively utilized in robotics to recognize objects in the robot's work area to provide additional safety measures by preventing collisions with objects within the area.[5,6]

Researchers could pursue many different approaches to laboratory automation. The approaches to automation can be divided into two main groups: process automation in the form of chemical reactors[7] or the use of robotic technologies in the form of cobots and industrial robots. Collaborative robot (cobot) is a collective name for robotic devices with built-in safety features (torque and momentum sensors), which makes them a perfect tool for laboratory automation due to the nature of chemistry equipment.[8] Typically, industrially manufactured cobots are presented in the form of articulated robotic manipulators.

A number of articles have been published that provide an overview of cobots and their application areas. For example, Taesi *et al.* reviewed a large number of literature sources to compare cobot solutions and provide an extensive market analysis.[9] Their article covers the technical aspects of collaborative articulated manipulators. This paper mainly focuses on reviewing several cases and methods related to CV and cobots that research teams around the world are using to conduct laboratory automation. We aimed to present state-of-the-art robotic solutions that have been developed and implemented in the field of chemistry. Table 1 summarizes the reviewed research articles that include cobots and CV applications in laboratory automation.

Automation of chemical laboratory

MacLeod *et al.* developed a self-driving laboratory (SDL) called Ada that uses two robots to synthesize and characterize thin film samples.[10] Robot N9 is equipped to mix, drop-cast and anneal precursors to create thin film samples. It also performs imaging and conductivity measurements. Robot UR5 can transport samples to additional modules, including an X-ray fluorescence (XRF) microscope. In their work, a camera was used as a tool to collect sample images for subsequent analysis. The robot positioned samples 90 mm below the camera and acquired visible-light photographs of each sample before and after annealing. Using this approach, a Pareto frontier map was developed linking film processing temperature and conductivity (Figure 1). The self-guided lab, driven by a multi-objective optimization algorithm called *q*-expected hypervolume

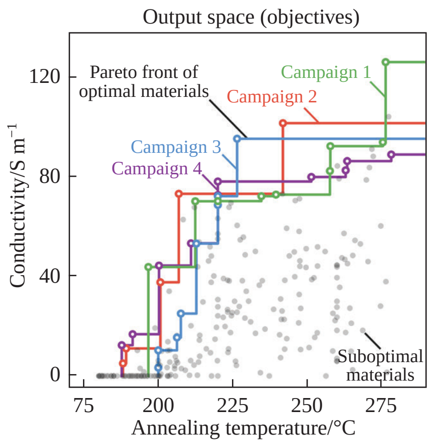

Figure 1 Determination of optimal conditions for low-temperature synthesis of sputter coatings on palladium films in a dedicated autonomous laboratory using an SDL equipped with a stationary robotic arm. The qEHVI algorithm quantified the trade-off between film conductivity and annealing temperature, generating an experimentally observed Pareto front (solid lines). For this purpose, an autonomous optimization campaign was run four times in a closed loop. Experimental points defining the fronts are marked with open markers, and selected points that are not part of the Pareto front are shown in gray.[10]

improvement (qEHVI), made it possible to identify synthesis conditions that can be adapted for a scalable sputter coating method capable of depositing high-quality, highly conductive palladium films at temperatures above 190 °C.

Burger *et al.*[11] propose to use a mobile collaborative robot KUKA KMR iiwa 14 to create an autonomous chemical laboratory for the autonomous search for the best photocatalysts for hydrogen production from water. This approach allowed the authors to conduct 688 experiments over eight days of continuous automated operation (Figure 2). The photocatalyst chosen for the study was the conjugated polymer P10, which exhibits high efficiency in the hydrogen evolution reaction (HER) in the presence of triethanolamine. First, the robot evaluated 30 candidate hole scavengers using a screening method without artificial intelligence. This revealed the potential of L-cystine as a reversible redox shuttle in the overall water splitting scheme. An autonomous robotic search was carried out on five hypotheses to accelerate HER. As a result, by selecting useful components and rejecting negative ones, this search revealed photocatalytic

Table 1 Summary of the use of collaborative robots and detection methods in modern research papers.

Field of study	Reference	Using CV	Main goal and tasks	Methods and equipment
Investigation of film conductivity and processing temperature	10	–	Synthesis and characterization of thin film Collection of images of the sample before and after annealing for subsequent analysis	Robots (N9 and UR5e) XRF microscope FLIR Blackfly S USB3 vision camera
Search for improved photocatalysts for producing hydrogen from water	11	–	Autonomous search for the optimal composition of photocatalytic hybrid material for efficient hydrogen production from water	Six-point calibration with respect to the black location cube Batched Bayesian search algorithm Robot (KUKA KMR iiwa 14)
Testing solubility in a solid–solvent system	12	+	Checking the solubility of substances Studying the transparency and degree of turbidity of solutions	Open-source Python package HeinSight Robot (N9)
Solubility testing and recrystallization	14	+	Determination of solubility of substances Measurement of turbidity of solution Detection of chemical glassware and assessment of its position	AprilTag as visual tags OpenCV for detection HeinSight for turbidity monitoring and measurement
Multiview perception of transparent objects	15	+	Interaction of a robot with a transparent object Perception of a transparent object	Depth estimation, segmentation and pose estimation using stereo camera ResNet-50 and 3D CNN neural networks
Robotization of the process of synthesis and analysis of a graphene oxide-based membrane	16	+	Empowering a robotic manipulator to use a centrifuge Determining the position of a centrifuge rotor using CV	ABB integrated computer vision COGNEX camera

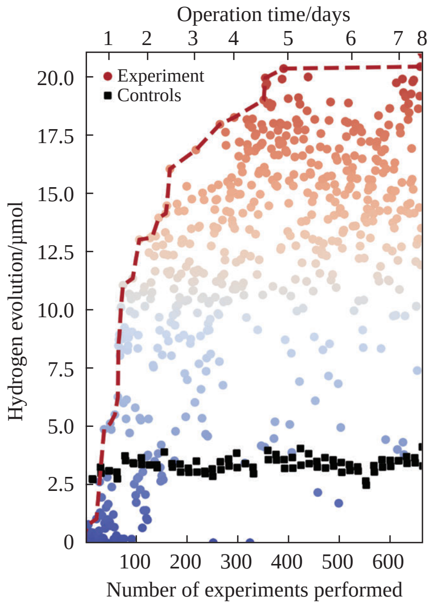

Figure 2 Determination of the optimal composition of the P10 photocatalyst for hydrogen evolution from water, performed by the automated SDL operation. The robot explored the chemical space to optimize the activity of the photocatalyst–scavenger combination based on five different hypotheses, performing 688 experiments. The graph shows the hydrogen evolution achieved during the offline search experiment. The black squares represent the baseline hydrogen evolution of 3.36 ± 0.30 μmol. The color transition of the dots from blue to red indicates an increase in hydrogen evolution.[11]

mixtures based on the P10/L-cysteine system that were six times more active than the initial formulations. However, the authors did not use CV algorithms to understand the robot's location in space, since the work took place in a dark room with light-sensitive samples. Instead, they used a six-point calibration concerning the black location cube and a batched Bayesian search algorithm for optimal parameters.

Shiri *et al.* used CV to automate a fundamental chemical experiment in materials synthesis, solubility screening (Figure 3).[12] The object of study was caffeine in various transparent solvents. The average brightness of all pixels in the monitored area was used as an indirect indicator of turbidity. This is a simple and inexpensive method for estimating relative turbidity with minimal computational effort. However, the study requires a white or light-colored solution and a transparent solvent. To achieve this, they developed HeinSight, an open-source Python package. The code reads images captured by a webcam and analyzes the pixels to obtain a proxy value for turbidity. The output value of the algorithm is then compared with an image of pure solvent to determine whether dissolution has been completed. The HeinSight turbidity code has also been used in other studies to determine when a solute has dissolved.[13,14]

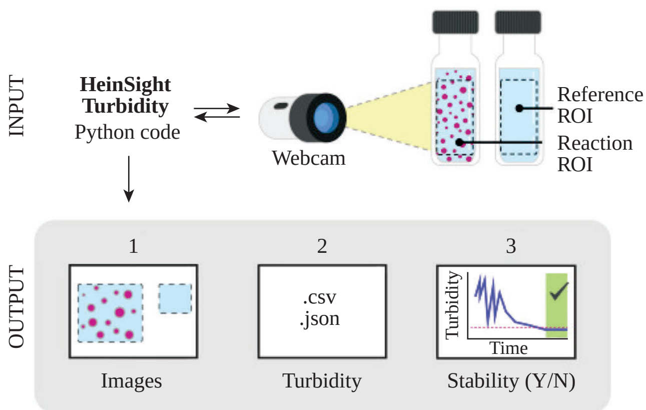

Figure 3 A robotic system based on a webcam for measuring turbidity using CV methods. The HeinSight turbidity code captures images from the webcam and analyzes the pixels in a predefined region of interest (ROI) to produce a proxy turbidity value. In the graph, control lines are represented by the dashed red line, and stability regions are shaded in green.[12]

Wang *et al.*[15] propose to use CV to recognize transparent objects for robotic manipulation tasks in home and laboratory settings. This task is critical in automation processes since transparent containers and reagents are often used in chemical laboratories. From a safety perspective, the robot's ability to recognize these objects helps to avoid accidental spills or mixing of reagents, which can lead to dangerous situations. Transparent objects can contain important information about the contents (*e.g.*, solution concentration), so robots that recognize such objects can more accurately perform tasks related to dispensing and mixing substances. Therefore, solving such a task will minimize errors in data collection and provide more reliable results. Their proposed method, MVTrans, is an end-to-end multi-view architecture with multiple sensing capabilities, including depth estimation, segmentation and scene understanding (constraint 3D frame and pose estimation).

As a result, a large photorealistic Syn-TODD dataset was collected for pre-training neural network models.

A similar application of CV is demonstrated by the work of Yoshikawa *et al.*, who described the use of a collaborative articulated robot (Panda) in solubility and recrystallization problems, *i.e.* fundamental chemical experiments in materials synthesis.[14] Their robotic platform takes as input an abstract description of a chemical experiment, then perceives the working environment using a camera attached to the robot gripper, a library with fiducial markers (AprilTag) and the OpenCV library, and then autonomously plans its tasks and movements using the PDDLStream solver.

CV software based on machine learning and neural networks

One of the main advantages of using CV in chemistry is the automation of experimental data acquisition and analysis. Traditional analytical methods such as spectroscopy or chromatography require a significant investment of time and effort, whereas CV enables real-time analysis. This not only speeds up the process, but also allows for analysis based on indirect parameters, since CV and neural networks are sensitive to changes in the system and can be trained to highlight specific experimental factors. For example, the group of Skorb *et al.* developed a method for determining the concentration of alcohol in a water–alcohol mixture using pre-trained convolutional neural networks.[17] The analysis was based on indirect data, namely, video recordings of the behavior of cavitation bubbles captured by a high-speed camera. This approach is based on changes in the shape, lifetime and velocity of cavitation bubbles with changes in the density and viscosity of the liquid. The use of transfer learning[18] reduced the amount of data needed to train the model. Despite the high required computing power, the use of the VGG network architecture[19] allowed for real-time analysis. As a result, a model was developed that can distinguish between five concentrations of alcohol in a water–alcohol mixture with an accuracy of more than 90%. A diagram representing the distinguishable cavitation bubbles in a water–alcohol solution in the alcohol concentration range from 0 to 25% is shown in Figure 4(*a*).

Additionally, the use of CV enables the control and management of chemical processes. Automation of a chemical process creates a system free from human errors.[7] Such systems allow continuous experimentation with varying input parameters, which helps in collecting data that can provide a comprehensive description of the chemical process. Continuing their research, the group of Skorb *et al.* improved their algorithm by applying a

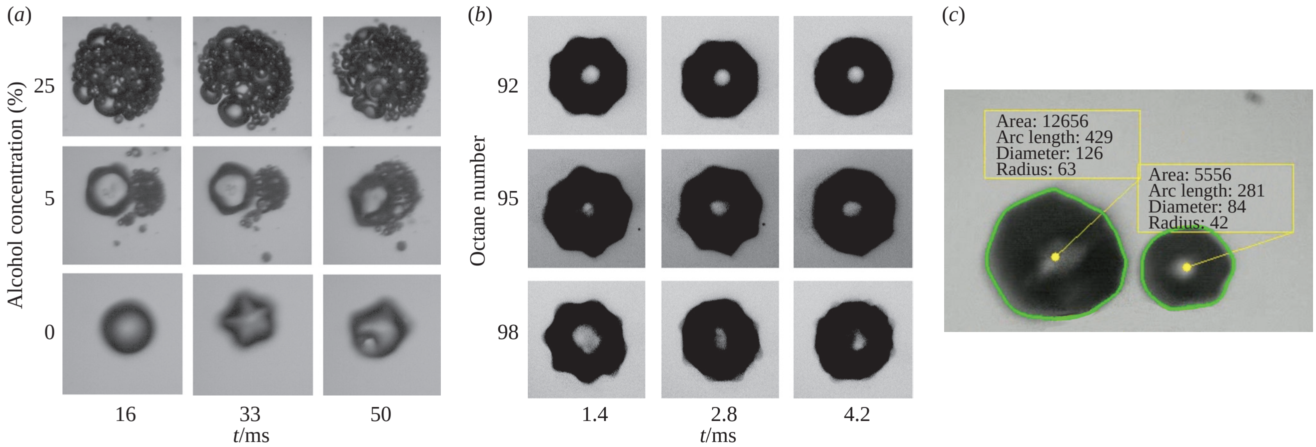

Figure 4 Images of cavitation bubbles in (*a*) an alcohol–water solution[17] and (*b*) gasoline[21] recognized using the classification algorithms. (*c*) Real-time snapshot of bubbles in gasoline processed using the segmentation algorithm.[21]

lighter ResNet architecture[20] and tested their approach to determine the octane number of gasoline.[21] The approach showed high efficiency, judging by the results presented in Figure 4(*b*); however, it did not allow tracking the state of the bubbles in real time. This feature could help to estimate the purity of the liquid and predict the presence of potential additives in the future with proper data storage and analysis. Both classical CV and neural network models such as YOLO,[22] SAM[23] and Mask R-CNN[24] can be used to implement this approach. Since classical CV algorithms do not provide sufficient accuracy in detecting cavitation bubble cluster formations, the YOLOv8 model was used. The trained model can determine the coordinates and sizes of bubbles in each frame, and if a video is available, it can track the bubbles in real time, as shown in Figure 4(*c*). To use the model, a web interface was introduced that allows the analysis of pre-recorded videos, as well as screenshots, to obtain and analyze data from the device in real time.

Detailed overview of the automated membrane synthesis laboratory

Separation of components, purification and concentration of samples are integral stages of many chemical and biochemical studies. These processes are performed using centrifugation.[25] For example, when obtaining quantum dots, this method is used to separate the particles of the dispersed phase of a colloidal solution after synthesis; in the production of drugs, centrifugation achieves the separation of sediments or other waste.[26,27] Several parameters can be varied during the centrifugation process, including the rotation speed and centrifugation time. These parameters can be adjusted depending on the specific requirements of the experiment or process. By varying the rotation speed, it is possible to control the force with which the particles are separated from each other. Changing the centrifugation time can affect the degree of separation of components. Skillful control of these parameters is critical to achieve the best results and the successful implementation of the centrifugation procedure. In this regard, automation of this method will allow the scientist to focus on more vital and non-trivial tasks. It will also increase the efficiency and accuracy of chemical research.

In the automated synthesis and analysis of graphene oxide (GO) and polyethyleneimine (PEI) membranes, CV was used to determine the position of the centrifuge rotor so that the ABB YuMi cobot could perform centrifugation during the membrane synthesis.[15] Since the membrane is prepared in excess polyelectrolyte, after centrifugation, all the polyelectrolytes are precipitated and react with GO, while the excess PEI remains in solution. Our research team has carried out this work, and therefore, some insights can be gained into the implementation of CV and the limitations of using the cobot.

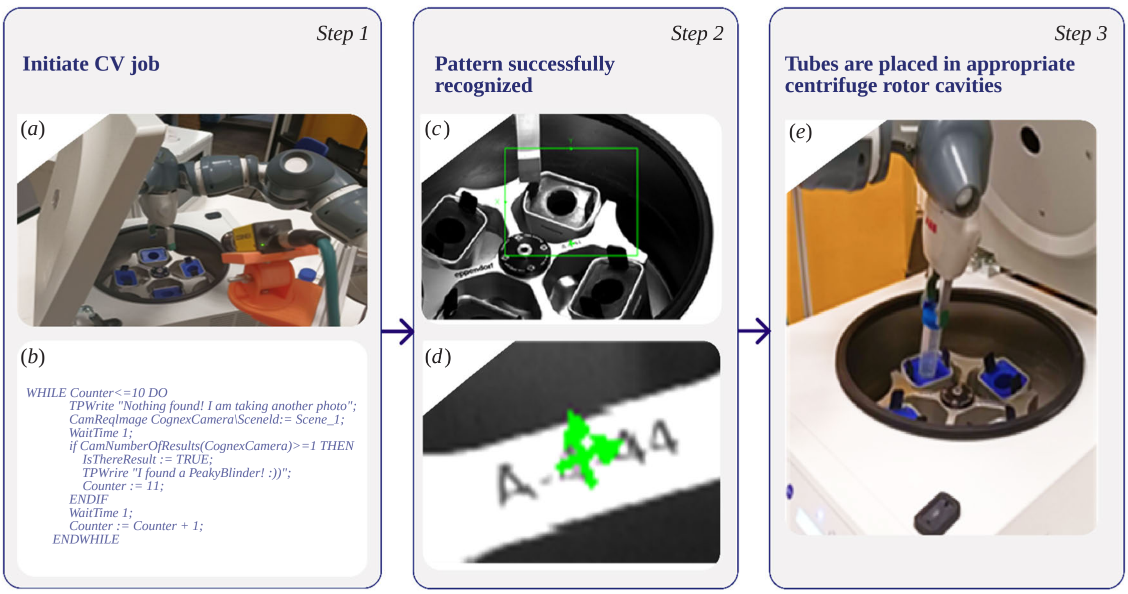

Figure 5 (*a*) COGNEX camera mounted on a desiccator stand. (*b*) RAPIDcode from the main script that initiates the pattern recognition job. (*c*) Image captured by the camera. (*d*) The pattern on the centrifuge rotor calculates the rotor position. (*e*) The robot places the tube into the centrifuge rotor.

During the development of the laboratory platform, several constraints were imposed. Since the laboratory platform was designed to be located in a shared laboratory environment, the development team was prohibited from modifying the specialized laboratory equipment of the centrifuge. Extensive safety features such as soft arm elements and precise momentum sensors were the determining factor in choosing the ABB YuMi robotic manipulator as the tool to perform the membrane synthesis and analysis process; however, this limited the maximum payload weight to 0.5 kg or 5 N of applied force (when the applied momentum exceeds the allowed range, an error occurs, requiring manual control). To overcome the limitation of the centrifuge rotor, a CV system based on a COGNEX camera and RobotStudio Integrated vision was implemented. As a first solution, it was decided to place the camera on the robotic arm.

However, this approach was deemed flawed due to the extra load on the end-effector, which resulted in false collision detection by the safety system and reduced detection accuracy. To mitigate this issue, a unique mount was designed to place the camera on the desiccator stand, as shown in Figure 5(*a*). The described CV system identifies markings [Figure 5(*c*)] on the centrifuge rotor to determine its position relative to the pre-programmed points [Figure 5(*d*)], which are used to set the laboratory tubes in the corresponding positions. Image recognition was implemented by training a feed-forward neural network in the RobotStudio Integrated Vision tool. It was called during the main routine using a specifically written procedure, as shown in Figure 5(*b*).

After successfully recognizing the marking, the ABB YuMi cobot proceeds to manually move the rotor to its destined position and then places the laboratory tubes into the centrifuge, as shown in Figure 5(*e*).

Conclusion

This review shows that there are currently many approaches to laboratory automation. Cobots using CV technologies can significantly improve the yield and quality of experimental data; however, there are several limitations and nuances to consider when designing a laboratory automation solution. As mentioned earlier, such nuances may include increased safety requirements due to the collaborative nature of automated chemical research laboratories, which directly impacts design choices, such as the type of robot used, the introduction of additional safety features and the design of the robotic tool; and surrounding area restrictions when conducting experiments that require special area conditions (light-sensitive or sterile laboratory cellular and biological experiments).

The above challenges are specific to laboratory automation, since such a rapid growth in the number of solutions for automated laboratories requires a new type of specialist who is proficient in robotics and understands the specifics of chemistry.

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