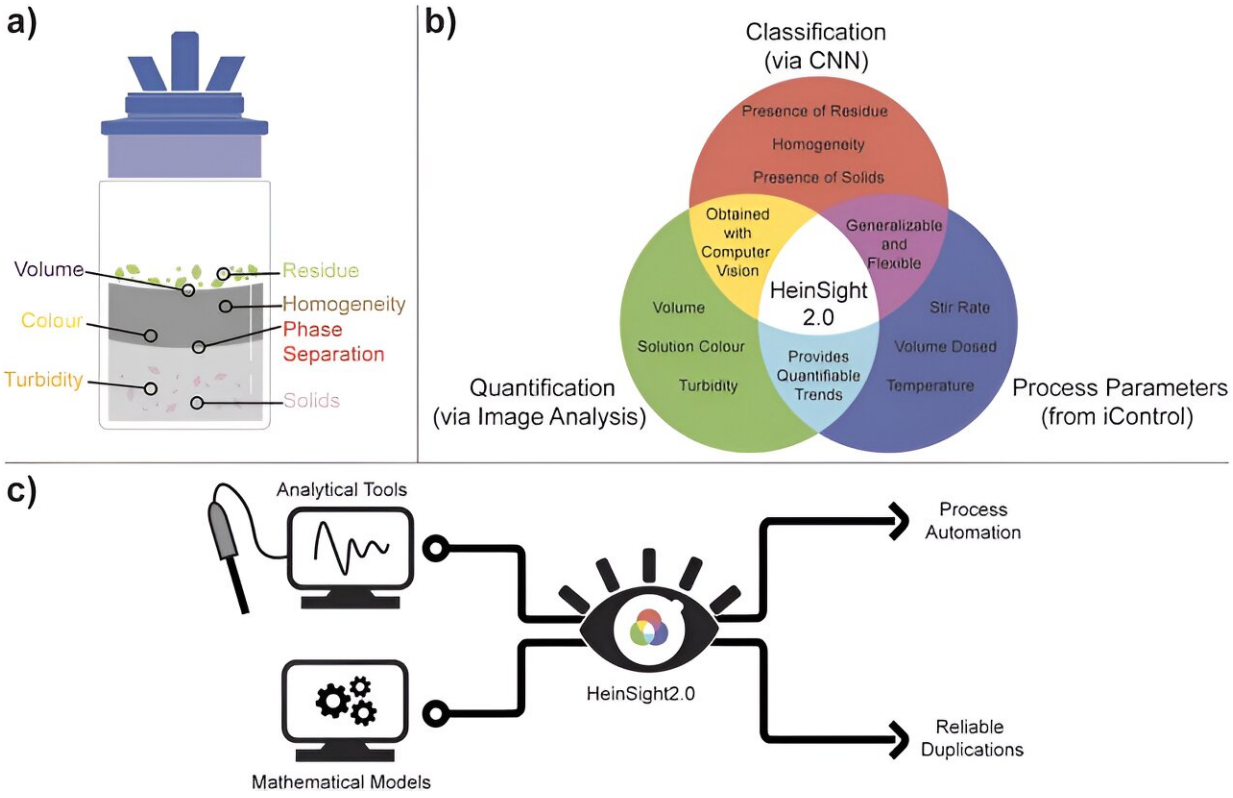
A computer vision and machine learning system that monitors and controls workup processes

January 8 2024, by Bob Yirka



(a) Universal vision-based outputs in workups monitored by HeinSight2.0; (b) overview of interrelated components of HeinSight2.0: Classification outputs (from CNN), quantification outputs (from image analysis), and process variables from iControl; (c) integrations and applications of HeinSight2.0 CV system. Credit: *Chemical Science* (2023). DOI: 10.1039/D3SC05491H

A team of chemists and engineers at the University of British Columba working with colleagues at pharmaceutical company Pfizer has developed a chemical processing system combining computer vision with a real-time machine-learning monitoring system for use in conducting chemical workup processes. Their paper is published in the journal *Chemical Science*.

In chemistry, workup processes are activities conducted to isolate a pure product through selective separation from other components. It is often tedious, which, besides being unpleasant, leads to mistakes or omissions. In this new effort, the research team has attempted to automate the process by combining computer vision with real-time monitoring techniques, a machine-learning system and computer processing, along with appropriate hardware, to carry out a workup process without assistance from human chemists.

The system developed by the team, called Heinsight2.0, as its name suggests, builds on knowledge learned from its predecessor, Heinsight1.0. Its components include a webcam (either overhead or side-mounted), reaction vessel, dosing unit, temperature probe and overhead stirrer. It also has a secondary device that allows for displaying iControl, real-time reaction trends, EasyMax and CV model output.

The system works by monitoring a workup process and controlling it by sending signals at appropriate times to direct the action as it happens. The system controls the action by responding as a chemist would as events unfold. If a material changes from one desired color to another, for example, the system can recognize that and use it as a cue to instigate a follow-up action.

The researchers note that, like a human chemist, the system is capable of monitoring multiple sensory cues and responding to them in desired ways. It can also operate under many types of scenarios, such as those

involving the use of solid-liquid mixing, crystallizations, exchange distillations and liquid-to-liquid extraction.

They also note that they have made the program script publicly available, which means other chemists could build their own units and then use the code to run their systems in the same way. They also plan to continue work on their system to give it more capabilities.

More information: Rama El-khawaldeh et al, Keeping an "eye" on the experiment: computer vision for real-time monitoring and control, *Chemical Science* (2023). DOI: 10.1039/D3SC05491H