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IoT-based electrosynthesis ecosystem

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ABSTRACT

In this paper, we presented the electrosynthesis ecosystem using esp8266 with OTA compilation integrated, the MQTT Broker for the control system that would be installed on a Raspberry Pi and MQTT protocol for the wireless data transfer layer which provides the electrosysnthesis machine to work 24/7 and with the AI that can be implemented, the whole ecosystem would be smart and the data-driven can be used in QC verification. This system is designed and simulated and the source codes are available via GitHub (https://github.com/iraniothome/ChemIoT).

1. Introduction

Lab work tasks can be tedious. Your time is too important for it to be spent watching an hour-long experiment just so you can manually adjust for example the temperature at the exact moment you need to. It's frustrating and prevents you from fully focusing on anything else at that time. With modern technology, you can automate your entire lab if you wanted to, from automated liquid handling and motorized pipettes through to robots labeling your samples and automated machines. The target of this paper is the automation of the electrosynthesis ecosystem.

Advantages of IoT-based chemistry ecosystem

1) **Scaling up the coulometry procedure to be used in industrial companies:** In fact, electrochemical methods possess many benefits over traditional reagent-based transformations, such as high functional group tolerance, mild conditions, and innate scalability and sustainability, simple, high sensitivity, comparable or better accuracy, cheaper instrumentation and lower cost of chemicals used, limited use of environmentally unfriendly organic solvents.
2) **Predictive Maintenance:** Advanced IoT technologies can help companies optimize their maintenance spends as well as minimize downtime.
3) **Energy Management:** Energy costs account for major production for Chemical companies. Monitoring energy costs is imperative for efficient operation. IoT can be put to use in this regard.
4) **Reliable results:** Chemists are judged on the quality of their chemistry. Automated chemistry systems enable you to precisely control reaction conditions, reducing the risk of human error and giving you greater confidence in your results.
5) **Increased productivity:** Chemistry experiments often involve lots of small adjustments throughout. Automated chemistry systems make these adjustments for you, enabling you to get on with other priorities or experiments. Create complex multi-step recipes to tell the software exactly when you want the temperature, stirring, dosing, or other variables to change. Save your recipes for re-use and standardize your workflows.

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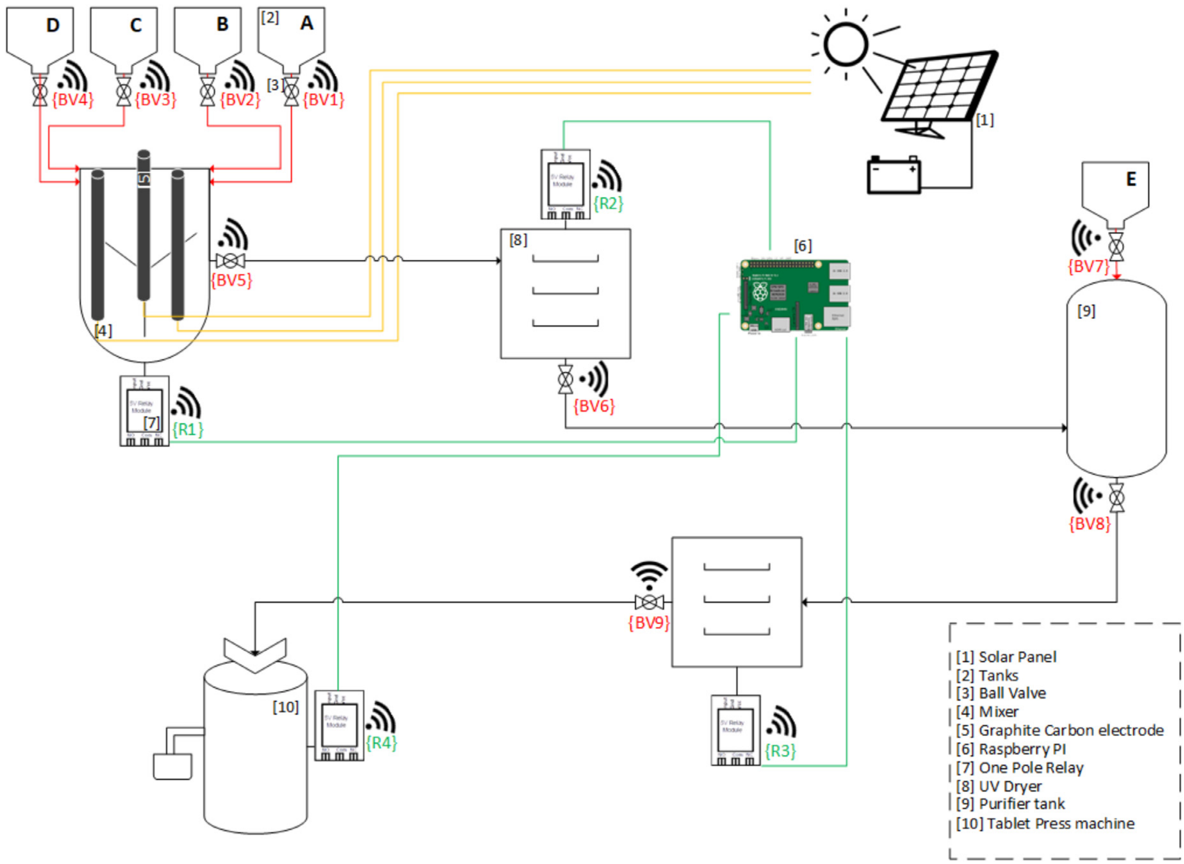


Scheme 1. schematic of IoT-based Electrosynthesis ecosystem.

6) **Safer working conditions:** Automation reduces the risk of accidents in your laboratory. Set limits that allow the system to shut down automatically if conditions are exceeded and set alarms to warn you when there is a risk of an accident.
7) **Save money, time, and lab space:** Automated chemistry systems cost more than manual systems and some are put off by that. But chemists who look beyond the initial expense are often convinced a switch is a right choice because they ultimately save money, time, and lab space.

For all the reasons mentioned above, wireless automated technology is not only an attractive choice in renovation and refurbishment, but also for new installations. Schemes 1–4

2. Experimental

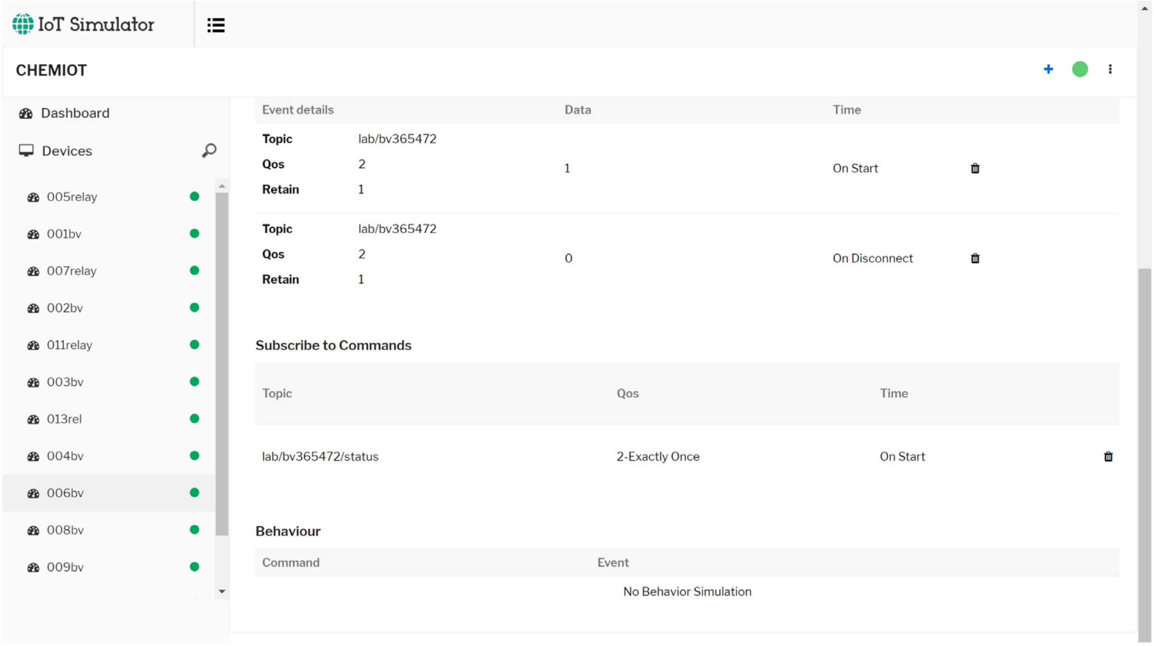
2.1. Materials and methods

Coulometry is based on an exhaustive electrolysis of the analyte. By exhaustive we mean that the analyte is completely oxidized or reduced at the working electrode or that it reacts completely with a reagent generated at the working electrode. There are two forms of coulometry: controlled-potential coulometry, in which we apply a constant potential to the electrochemical cell, and controlled-current coulometry, in which we pass a constant current through the electrochemical cell. Based on the published paper [1], in this project, we use controlled-potential coulometry.

IoT-based Electrosynthesis ecosystem steps

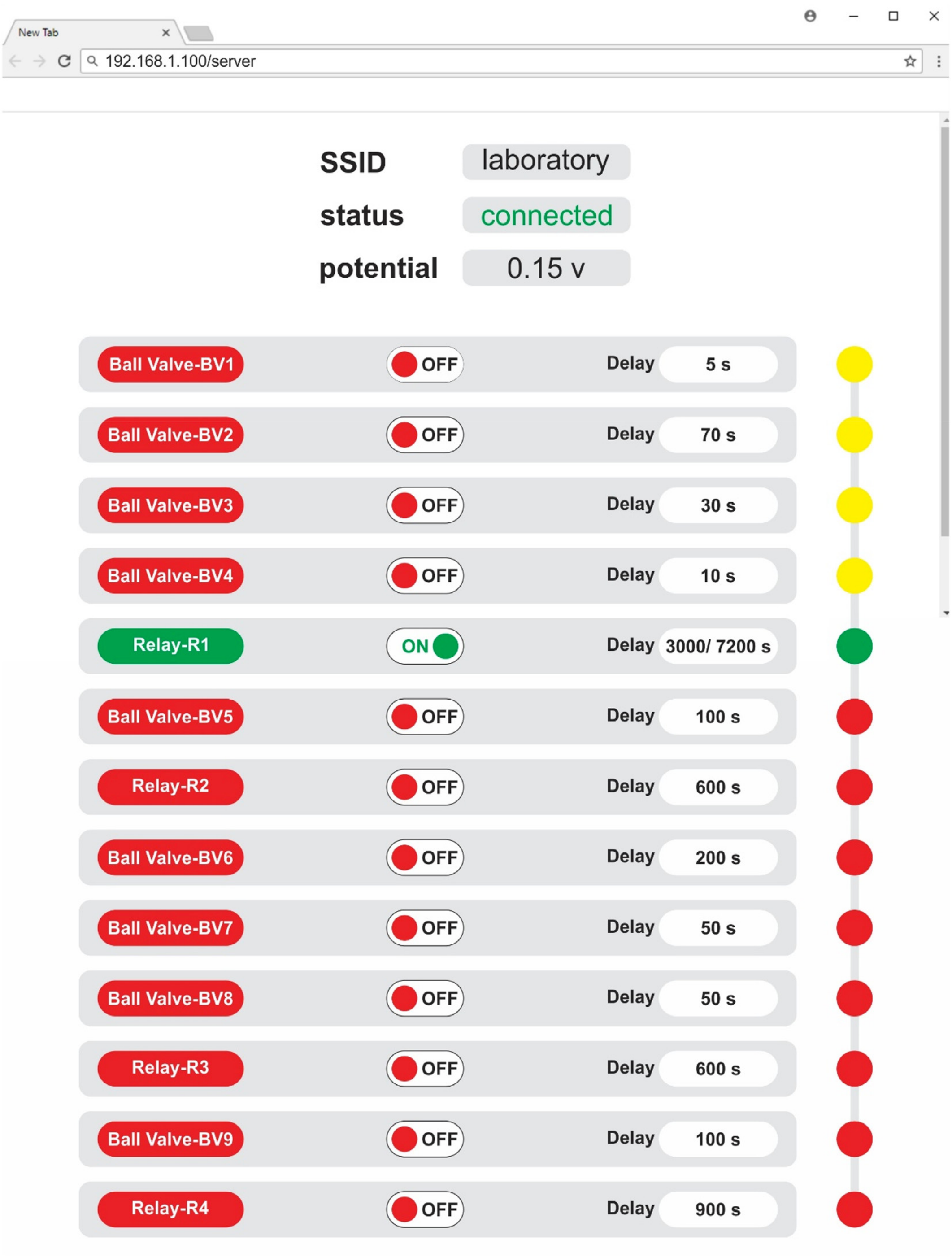
The procedure steps would be as follow:

1- The Solar panel would support and produce the energy of all the infrastructure motorized ball valves but for the control of the valves we use battery powered NodeMCU attached to the One pole Relay and connected to the motorized ball valve. All the hardware modules can be compiled over the air (OTA) and can connect to the SSID through the Smart-Config library of the esp8266 and all the data logs would be saved in JSON files. The sample code which is implemented in the esp8266 would be available on the Github profile.



Scheme 2. Simulated network and example pub/sub topics.

2- The automated ball valve connected to the RPi MQTT broker and controlled using WiFi and MQTT IoT protocol. Each esp8266 would be unique and identified with the special equation.
3- Based on this certain chemical procedure, the tank A would be filled with the specified amount of substance A. Then the remotely managed ball valve BV1 would be set to ON and let the substance A pour into the Mixer.
4- The tank B, C, and D would be filled with the specified volume of substances B, C and D Then the IoT- based ball valve BV 2,3 and 4 would be set to ON and let the other substance pour into the Mixer.
5- The relay R1 that attached to the mixer would be set to ON via MQTT topic or automatically as all the 4 ball valves set to OFF after a short delay; the publish command would be lab/bv + clientID which turns the digital pin to HIGH via the topic payload of 1. concurrently the solar-panel would support the energy needed for the graphite carbon electrodes. In this case, the potential needed is 0.15 V.
6- After the programmed delay which is needed to complete the redox process (a quantitative electrolysis by using an electrode with a large surface area, and with a high stirring rate typically requires approximately 60–120 min, although shorter or longer times are possible); the ball valve BV5 would be set to ON and the mixture would be transferred to the UV dryer via gravity.
7- The programmed and remotely relay R2 would set the UV dryer status to remain ON for near 15 min. All the hardware are subscribed to the lab/bv + Client ID/status command to get the status.
8- After the time mentioned above, the IoT-based ball valve BV6 would be set to ON and let the powder remained from the mixture solution, transfer to the purifier tank via gravity and after a specific amount of time, it goes back to OFF, the status would change and the module goes to deep sleep mode for saving battery.
9- The tank E would be filled with substance E and as before, the IoT-based ball valve BV7 would be set to ON and let the substance E (in this chemical procedure, $CH_3CN/NaOH$) pour into the purifier tank. [1]
10- In the purifier tank, the precipitated solid was washed with acetonitrile and NaOH for separation of the remaining substances.
11- The ball valve BV8 would be set to ON after almost no delay and let the purified solution transfer to the next dryer via gravity and after a short delay, sets back OFF.
12- Relay R3 which is connected to the UV dryer would be set ON manually and works for around 15 min or automatically after the ball valve BV8 is done (OFF).
13- After the programmed delay which is needed for the UV dryer, ball valve BV9 would be set to ON and let the finalized product which in this specific method is Indole powder [1], transfer to the tablet press machine and set back to OFF after a short delay. In this state, we have pure indole. Indole derivatives have been a topic of substantial research interest and continue to be one of the most active areas of heterocyclic chemistry, particularly due to their natural occurrence and pharmacological activities [2]. Indole and its homologs are found in coal tar [3] and in molasses tar. Indole nucleus is also found in tryptophan (an important nutritional constituent), plant hormones, and certain important alkaloids [3], as well as in liver [4], pancreas [5], brain [6] and bile [7]. In addition, indole is a powerful

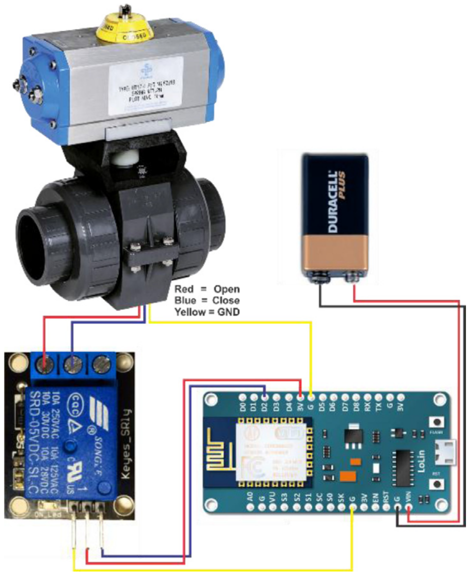


Scheme 3. MQTT dashboard UI/UX.

anti-oxidant, and it appears to be especially effective against breast and cervical cancer because of its ability to increase the breakdown of estrogen in the human body [8]. On the other hand, regarding the increase in the importance of green chemistry in organic synthesis, development of more efficient and environmentally friendly processes for chemical transformation is desired [9].

14- The relay R4 which is connected to the tablet press machine would be set to ON after the ball valve BV9 is done or manually to produce tablet and capsules.

Based on the procedure above, the schematic of the MQTT broker installed on RPI would be as follow:



Scheme 4. The module.

3. Result and discussion

Based on the chemical procedure that has been done before in the co-author's paper [1], the current methodology to produce indoles as a cure for the women cancer diseases has not been industrialized yet and with the ecosystem provided here, it can be commercialized and industrialized. Using MQTT broker installed on the Raspberry Pi in this method would help us to have the controller in the laboratory which can store the data collected from the procedure and for the further usages, we can implement the fog computing OS on the RPi to process the data and let the suitable ones upload to the main MQTT server for the connection of laboratories. The hardware we are developing here is going to be something like this.

The NodeMCU with the esp8266 SOC which is used in this paper is able to be compiled over the air via OTA library. Because the module is battery powered, it goes to DEEP SLEEP mode when transfers the data to the server, so the battery would remain for at least 2 years.

The MQTT protocol helps us to improve the QOS level of transferring the data and with the QOS 2 which is exactly once, we would be sure that the command has been delivered to the actuator.

4. Conclusion

Based on the reference paper [1], the chemical procedure would lead to producing not only the purified indoles but also can be used to produce more substances such as Thiazole [10], Phenothiazines [11], Paracetamol [12], BenzoThiazole [13], Benzofuran [14] and based on the simulation installed on the RPi MQTT server, the IoT based automation method is working fine with full power and high accuracy and performance.

The other conclusion driven from this methodology is that integrating IoT and using data science to use the data-driven from this procedure would help us to automate not only this method but also all the laboratory and industrial machines to work 24/7 without any human interference and fault.

Conflict of interest

The vision is to achieve a method that affects the future of drug production companies, pharmaceutical industries, and laboratories based on the 24/7 remotely automated electrosynthesis ecosystem to produce more and purified tablets, drugs and other substances mentioned above for the human health.

References

[1] A. Asghari, M. Ameri, S. Radmannia, M. Rajabi, M. Bakherad, D. Nematollahi, J. Electroanalytical. Chem 733 (2014) 47–52.
[2] J.A. Joule, K. Mills, Heterocyclic Chemistry, Blackwell Science, Oxford, 2000.
[3] R. Weissberger, Chem. Ber 43 (1910) 3520–3525.
[4] N.A. Shafakat, B.A. Darab, V. Pradhana, M. Farooquia, Mini. Rev. Med. Chem 13 (2013) 1792–1808.
[5] M. Nencki, Chem. Ber. 7 (1874) 1584–1593.
[6] F. Stockly, J. Prakt. Chem 24 (1881) 17.
[7] C. Ernst, Physiol. Chem 16 (1892) 208.
[8] D. Nematollahi, V. Hedayatfar, J. Chem. Sci 123 (2011) 709–717.
[9] R. Ojani, J.B. Raoof, R. Hosseinzadeh, A. Alinezhad, Montash. Chem 140 (2009) 503–508.
[10] M. Ameri, A. Amoozadeh, A. Asghari, D. Nematollahi, M. Bakherad, J. Helvetica (2015) 210–223 98.2.
[11] O. Ghaderi, A. Asghari, M. Ameri, M. Rajabi, J. Chem. Soc. Jpn 45 (2016) 430–432.
[12] A. Asghari, M. Ameri, A. Ziarati, M. Rajabi, S. Radmannia, A. Amoozadeh, J. Chin. Chem. Lett. 26 (2015) 681–684.
[13] M. Arab, H. Daneshinejad, M. Bakherad, M. Ameri, J. Croatica Chemica Acta (2016) 7–15 89.1.
[14] M. Rajabi, S. Radmannia, M. Ameri, A. Asghari, M. Bakherad, J. Progr. Reaction Kinetics Mech. 40 (2015) 163–168.