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Next-Generation Polymerization: Precision Automation Meets Smart Material Discovery

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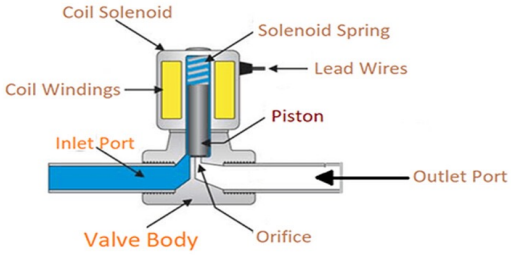
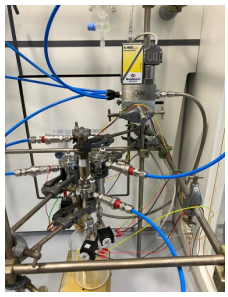
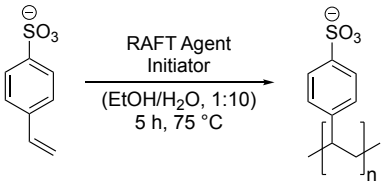
Introduction – Digitized chemistry

Artificial intelligence has revolutionized chemistry by streamlining processes and accelerating discoveries.[1] Through machine learning algorithms, AI predicts molecular properties, aiding in drug design and material science. Furthermore, it enables virtual simulations, reducing costly experiments.[2] However, AI-driven robotics automate chemical synthesis, enhancing efficiency and safety. Nonetheless, all automated dosing systems recognized in the literature suffer from the disadvantage of being highly susceptible to oxygen and humidity, greatly limiting their practical usefulness.[3] In this work, we present the first automated dosing system capable of conducting polymer chemistry under inert conditions.





Polymerization inside the reactor



Scheme 1. Polymerization of styrene sulfonate.

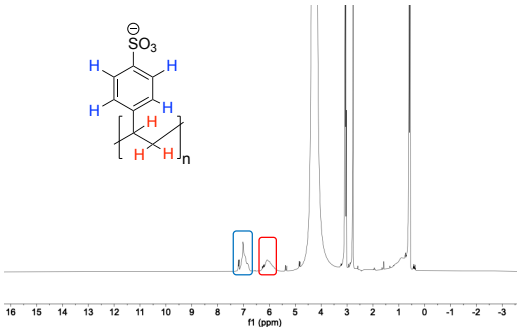
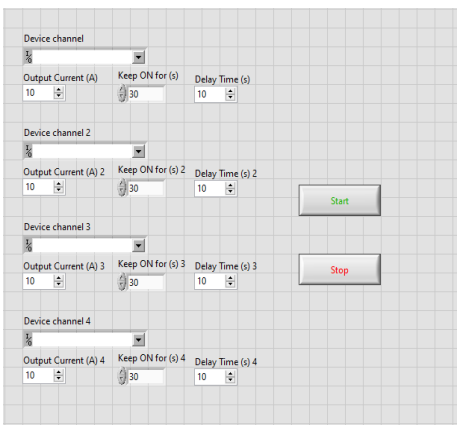


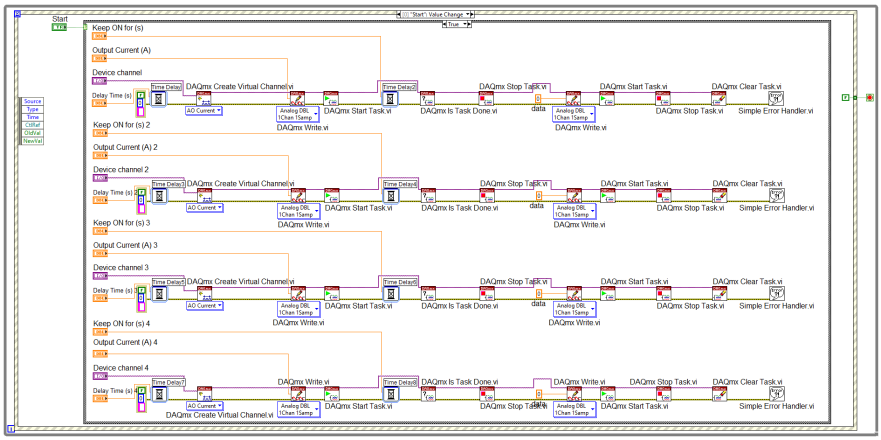
Figure 1. ^{1}H-NMR spectrum of the reaction solution of the polymerization.

Table 1. Molecular weight after the polymerization of styrene sulfonate.

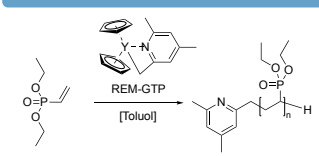
Experiment Number	M_n (kg mol^{-1})
1	40.8
2	40.5
3	40.3
4	40.4
5	40.2
6	40.3
7	40.4
8	40.5
9	40.4
10	40.3

Automation code using LabView





Future work



Supplementary polymer classes, such as vinyl phosphonates, will be synthesized to demonstrate the universality of the dosing system for a wide range of air- and oxygen-sensitive reactions. Furthermore, implementing an AI for complete automation and analyzation is planned. Hence, the AI will have the capability to operate the adjacent NMR device to analyze the completed polymer and to modify the reaction parameters or administer potential additional dosages of reactants to achieve customized polymers.

References

[1] Z. J. Baum *et al.*, J. Chem. Inf. Model. **2021**, 61, 3197−3212.

[2] For example – J. N. Kumar *et al.*, *npj Comput Mater* **2019**, *5*, 73.

[3] D. Caramelli et al., *ACS Cent. Sci.* **2021**, *11*, *1821−1830.*