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EDITORIAL

Meet The Flow Chemist – Prof. Ryan L. Hartman

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Name	Ryan L. Hartman
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1) When did you start with flow chemistry? Describe the first paper or the first experiments.

I started my career designing reservoir stimulation technology in the upstream petroleum and gas industry. Most operations in that industry are continuous-flow and the chemistry is complex, often involving both inorganic and organic reactions. We designed laboratory experiments routinely with packed-bed laboratory reactors in collaboration with computational experts to understand flow and reaction in porous media for field operations. Those experiences were foundational for my transition into fine chemicals and pharmaceuticals. In a paradigm shift while working with a fantastic team of gifted scientists and engineers at MIT, we laid important groundwork for what we know today as "flow chemistry". Learning about organometallic synthesis with a skillset of a traditional reaction engineer was truly a unique opportunity to innovate and rethink our approach to studying the physical and chemical rate processes.

2) What are the main benefits of flow that convinced you to use and implement this technology in your research?

The opportunity to study mechanisms is what first attracted me to design flow reactors with in-situ analytical methods. Many of the problems I was interested in as an independent researcher had been studied using outdated methods. Consequently, there were prospects to discover new science then and remain today, even in mature fields. Flow chemistry is a disruptive technology, and I think it has catalyzed the development of adjacent fields and probably also the creation of new fields. Beyond those examples, the advantages of performing experiments faster, generating more data, precision, energy and environmental impacts, and under conditions that the engineer can model all continue to motivate my interest in flow chemistry.

3) What do you think the future holds for flow chemistry?

I'm certainly not an expert in predicting the future, but I think digitization will play an important role. The synchronization of computers with experiments is transformative

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in the laboratory but also in manufacturing. Convergence of the science and engineering disciplines has already been demonstrated, and probably we can expect even more so as new materials and chemical processes are innovated. Sustainability in chemicals manufacturing continues to be of broad interest to academics and practitioners with many unanswered questions.

4) Do you have any relevant tips for newcomers in the field?

Don't be afraid to challenge the cultural norm or rethink conventional methods – it is why flow chemistry exists today. Take advantage of your background and skillsets – use first principles to discover or redefine. Teams composed of strengths in core areas who work together to solve problems also tend to be more effective than diluted expertise or individuals.

My three most relevant papers related to flow chemistry:

1) Liu, Y., Sabio, J., and Hartman, R.L. "A Counter-Current Flow Micro-Packed-bed DBD Plasmatron for the Synthesis of a Methylated Cobaloxime", J. Phys. D: Appl. Phys., 54, 194003 (2021).

Our findings report the design, modeling, and application of a multiphase, microplasmatron for the use of electricity-generated, low temperature plasmas for the direct methylation of a cobalt organometallic catalyst. In the context plasma physics, which is the fourth state of matter, the work demonstrates that "flash chemistry" can be studied with multiphase microplasmatrons, where transport limitations and electric fields in conventional reactor designs could be expected to influence the reaction outcome.

2) Rizkin, B.A., Shkolnik, A.S., Ferraro, N.J., and Hartman, R.L. "Combining automated microfluidic experimentation with machine learning for efficient polymerization design", Nat. Mach. Intell., 2, 200-209 (2020).

This paper reports the design of a semi-automated microreactor system to quickly narrow in on an olefin polymerization catalyst's activity for multivariate reaction conditions, including different temperatures and zirconocene-catalyst, activator, and monomer concentrations. The study exemplified the power of experiments and computations working together synchronously to generate information faster and with better accuracy than conventional batch techniques currently used in polymerization research and manufacturing.

3) Hua, T. and Hartman, R.L. "Computational Fluid Dynamics of DNA Origami Folding in Microfluidics", React. Chem. Eng., 4, 1818-827 (2019).

This paper challenges the state-of-the-art of batch techniques by answering the questions – should DNA programmable materials be studied with microfluidics, and if so, then why? Our findings demonstrate that the reactor type and the choice of single or multi-phase flows can be guided by the information desired (e.g., activity, kinetics, selectivity, or equilibrium conversion). The research also reports a theoretical model for the equilibrium folding kinetics of a DNA origami.