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\$15,000 "Use it!" Lemelson-MIT Student Prize Graduate Winner

Chemical reactors for more sustainable chemical processes and an optimized system for energy storage and hydrogen production

The Challenges: Every day we interact with products and materials manufactured by the chemical industry, from components in the cars we drive, to the clothing we wear. Chemical reactors, or the equipment used to convert raw materials into useful products, are key components of the chemical manufacturing process because they define the efficiency and sustainability of the chemical transformation. The chemical reactors used in current manufacturing processes are not sustainable because they use mostly heat from fossil fuels (i.e. thermal processes) and release large amounts of CO₂, making the chemical industry the third largest producer of greenhouse gases. An alternative is the development of electricity-driven processes (i.e. electrochemical processes), which are more efficient, can integrate renewable energy sources, and are more sustainable. One area where these options play a major role, is the production of nylon. Adiponitrile (ADN) is one of the main components that leads to the development of nylon 6,6. Nylon 6,6 is found in a wide array of products, such as automotive parts, firefighting gear, engineering plastics, and apparel. The demand for nylon 6,6 is constantly increasing due to its many uses, which is causing a worldwide shortage in the supply of nylon's intermediates, such as ADN.

The chemical reaction that produces ADN is the bottleneck in the nylon production process. The two current ADN manufacturing methods (thermal and electrochemical), are expensive, dangerous, and complex, making capacity increases difficult and costly, and supply unreliable, with frequent price increases. The thermal process uses high pressures, temperatures, and dangerous chemicals such as hydrogen cyanide, hindering its quick growth. Although the electrochemical route is scalable and more modular, the process is not well understood. It consequently suffers from large inefficiencies, low profit margins, and multiple complications. Furthermore, nylon

manufacturing is extremely unsustainable, releasing five times more energy than cotton manufacturing, causing more CO₂ emissions.¹

Another worldwide energy-related issue is that power grids are highly vulnerable to natural disasters, which often result in power outages across large geographical areas. Renewable energy storage systems could provide the backup necessary in emergency situations, however their availability is hindered by cost, scale, and the stationary nature of the developed technology. New engineering strategies are needed to improve the competitiveness and impact of clean energy.

The Solutions: Daniela's primary invention is a chemical reactor that combines pulsed electrical voltage and artificial intelligence (AI) optimization to enhance chemical processes. One of the largest chemical processes that could benefit from Daniela's reactor is the production of ADN, leading to the creation of more sustainable nylon-based materials, such as textiles. By using pulsed electricity to power the reactor instead of heat from fossil fuels, combined with machine learning optimization, Daniela's chemical reactors use 30% less energy, 30% less raw material, and produce 30% less emissions, all of which leads to a 20% reduction in manufacturing costs. The savings in energy and raw material transform the nylon production process, making it less expensive and more sustainable.

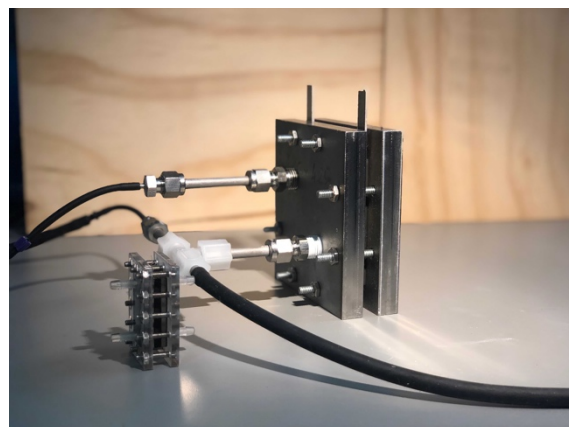


Figure 1: Prototype of chemical reactor invention.

This is a significant improvement over the current electrochemical process implemented at scale in industry, and could either be a drop-in solution to existing plants or an easily implementable solution to new ones. The invention is paradigm-changing as it's the first to implement machine learning algorithms in the optimization of electrochemical reactors. Daniela's chemical reactors and AI technology can be implemented in a variety of chemical processes, highly reducing the number of experimental data points. Her goal is to use this invention to make the chemical industry greener, one reaction at a time.

Daniela's secondary invention is a proof of concept of an optimized system for energy storage and hydrogen production. One side of the system is designed to release energy in the form of electricity, whereas the other side requires an electrical input to

¹ <https://oecotextiles.wordpress.com/2011/01/19/estimating-the-carbon-footprint-of-a-fabric/>.

produce hydrogen. Both sides can be operated independently, allowing users to take advantage of electricity prices, given that prices fluctuate throughout the day and year according to demand. When electricity prices are low, the user purchases electricity to run the side of the system that requires an energy input to produce clean hydrogen fuel. When electricity prices are high, the user runs the opposite side of the system and sells the generated electricity to the grid. This system makes clean energy storage cost-competitive, and the hydrogen produced can be used as a transportable energy carrier, readily available to address energy needs in areas affected by natural disasters and power outages.

Commercialization: Daniela co-founded Sunthetics, a startup that has raised over \$400K to scale up and commercialize her nylon production technology. Sunthetics is planning to enter the market as a supplier of easy-to-use and efficient electricity-driven reactors for more sustainable chemical processes in the pharmaceutical industry. The company will also offer the AI software and consulting services to lower the barrier to implementation of more sustainable electrochemical reactions. In parallel, Sunthetics will continue to scale up the reactors' production, reaching the capacities needed to license the technology in the nylon supply chain. Customers will include downstream nylon manufacturers with strong partnerships throughout the supply chain, specifically with eco-friendly outdoor apparel and performance wear brands that rely on large amounts of nylon in their production. The technology offered by Sunthetics will then be available to multiple sectors of the chemical industry (e.g. cosmetics, other textiles, petrochemicals) for the sustainable production of a myriad of chemicals at different scales.

Daniela has a patent for her second invention and it is available for licensing through New York University.