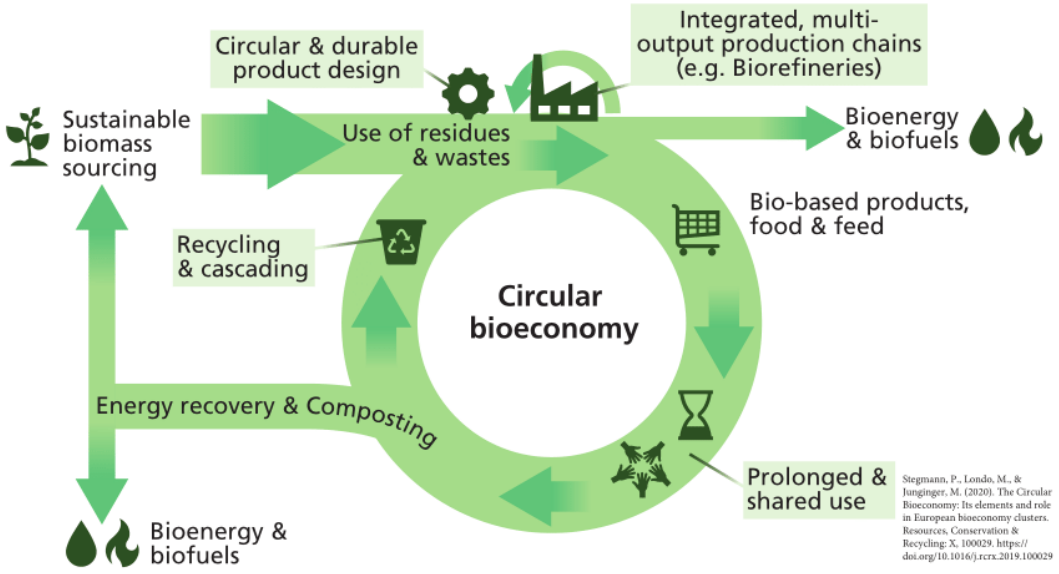
Why reinforcement learning is a good approach for obtaining global optimal in new (bio)chemical process design?

Introduction

The chemical industry is going through a transition into a sustainable and circular production of chemical products and energy. To accelerate this transition, new supply chains and manufacturing processes must be redesigned, with the objective to include new renewable raw materials like biomass, waste or even CO2 for producing chemicals products.



The remaining challenge: Fast and flexible flowsheet generation

For evaluating these new sustainable manufacturing alternatives, new flowsheets need to be designed and optimized to evaluate the up scaling of those biochemical processes, estimating the related costs and the life cycle assessment.

Due to the high dimensionality and the high number of possible options, the engineering of new processes is still currently based on previous processes, or engineer's intuition, which makes it difficult when having to extrapolate to new disruptive processes or adapt new raw materials / waste into existing flowsheets, leading to sub optimal designs.

To solve that problem, computed aided tools had been developed to optimize the whole flowsheet, using methods like MINLP or Genetic Algorithms. However, there are still some limitations with these tools: On the one hand, initial superstructure or subgroups (reaction, separation, purification) must be defined, which sometimes leads to suboptimal results.
On the other hand, each variable, its topology (discrete or continuous) and its boundaries must be defined, which also reduces the exploration flexibility. Third, in terms of computation, each experiment starts from scratch (without any previous knowledge), so it takes a long time to reach optimal designs for different scenarios (different feed compositions, different market prices, etc…).
Apart from those technical challenges, you must be an expert using numerical methods like Matlab and coupling it with process simulators like Aspen Plus (and dealing with errors…).

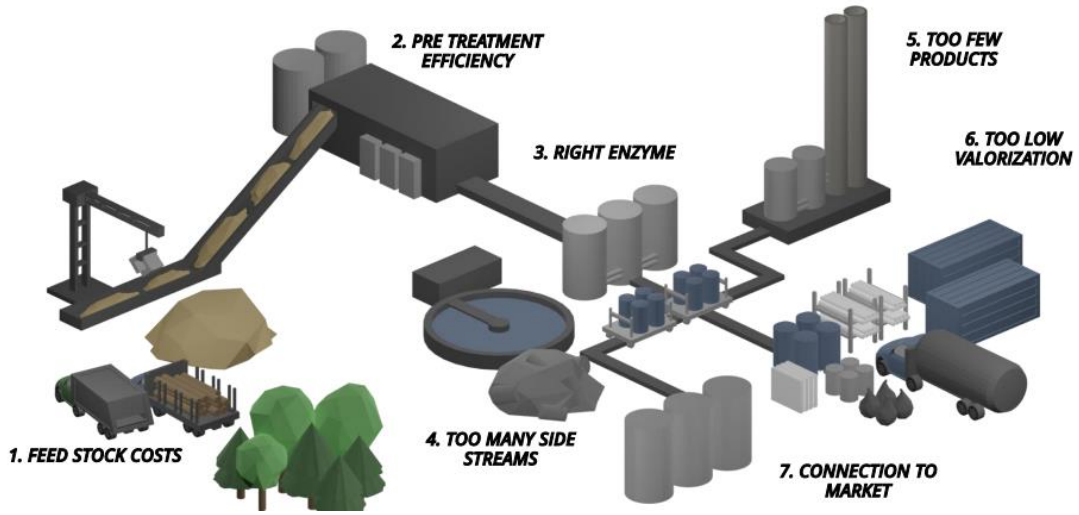


Figure 1. *The design of new biorefineries is complex and it often leads to sub-optimal results, among other things, because of the large number of streams and the need to obtain high-value side streams or waste recovery.*

Beyond performing simulations. Learning from them.

Reinforcement learning is an AI emerging technology that is promising in many fields which present complex optimization and involve sequential decision making, like videogames or other problems that have a massive combinatorial action space, measurable metrics, and an efficient simulator. But… What has this got to do with (bio)chemical processes?

All (bio)chemical processes on an industrial scale are based on multiple steps (conversions, separations, etc…), so it is not possible to optimize an entire process at once (like the shape of an airplane's wing, for example). The different steps are unit operations of the process:

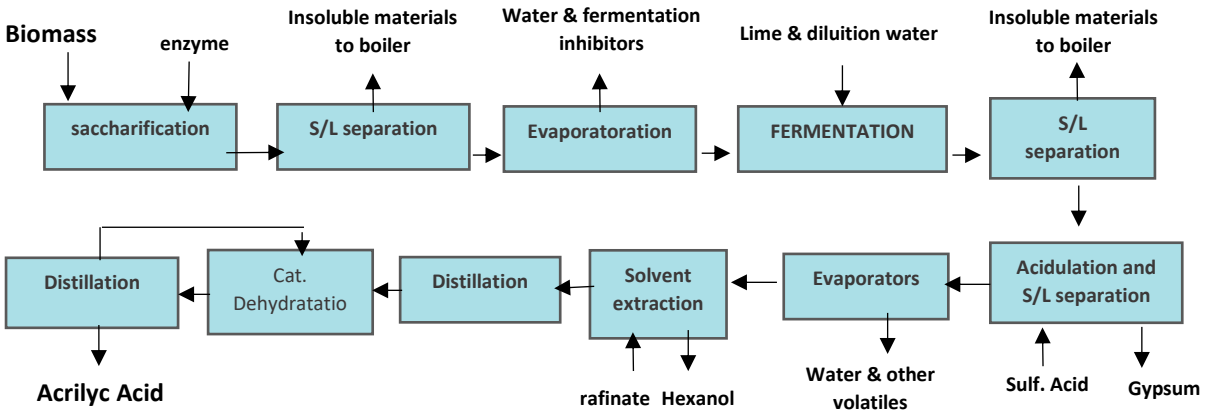


Figure 2. *Exemplar process of production of acrylic acid via fermentation.*

Reinforcement learning learns from sequences of actions or transformations, optimizing the route (or transition) from initial states (feedstocks) into an objective (valuable products).

So once Reinforcement learning (RL) is properly coupled to a process simulator (a virtual environment), it can be very powerful with the following decision making, needed to evaluate a potential (bio)chemical process on early stages:

- From my feedstock to valuable products. Which technologies do you recommend?
- Which unit operations will I need?
- What will be the CAPEX and the OPEX?
- Which is the life cycle analysis?

One of the capabilities that RL has is the ability to make open exploration. The engineer doesn't need anymore to define the boundaries of each variable in the optimization. RL learns by itself what's good and what's not, by navigating in the new space, through simulations, and learning which is the best route to follow.

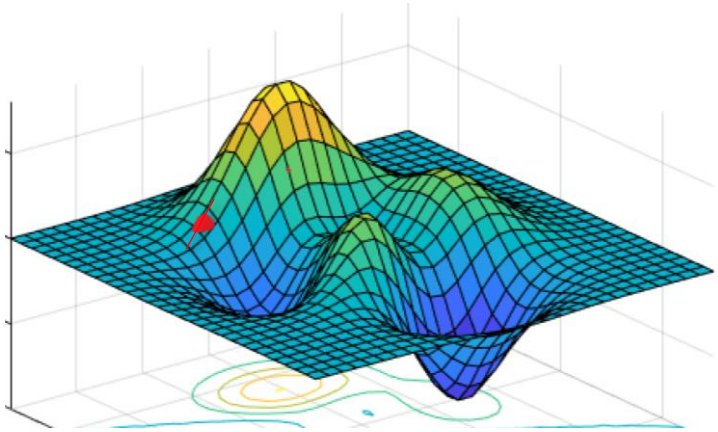


Figure 1. *Example image of a 2d stochastic optimization.*

In new process design, once the algorithm has performed thousands of simulations, RL has an idea of how to interact in the chemical space to produce the products of interest, which has complex rules like thermodynamics, kinetics, transport phenomena, etc… a much more complex space than this 2d graph image on top.

The learning from past experience is mathematically described by the Bellman equation, which is a Markov decision process, a typical algorithm in reinforcement learning.

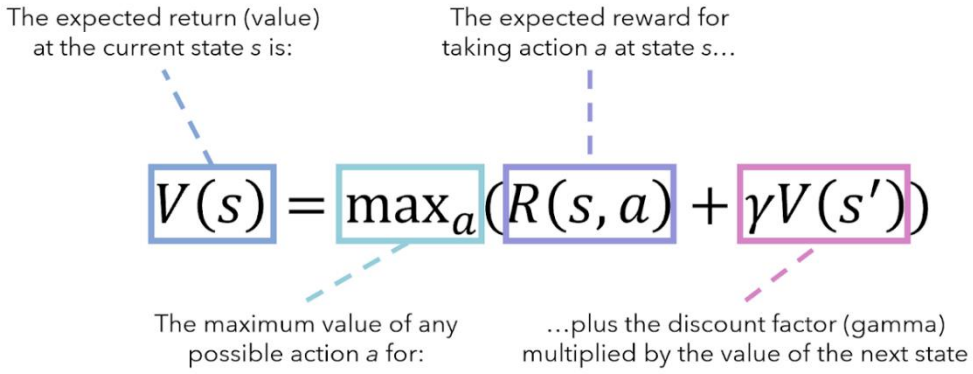


Figure 2. *The bellman equation estimates the probability for each possible action of being the best to perform, in a specific state (flowsheet current information), to obtain optimal performance at the end of the design.*

What if we could execute thousands or millions of simulations and learn from them? This was the value proposition of Intemic, which has been reflected in their proprietary software called "Flowsheet Copilot", which works as described in the following scheme:

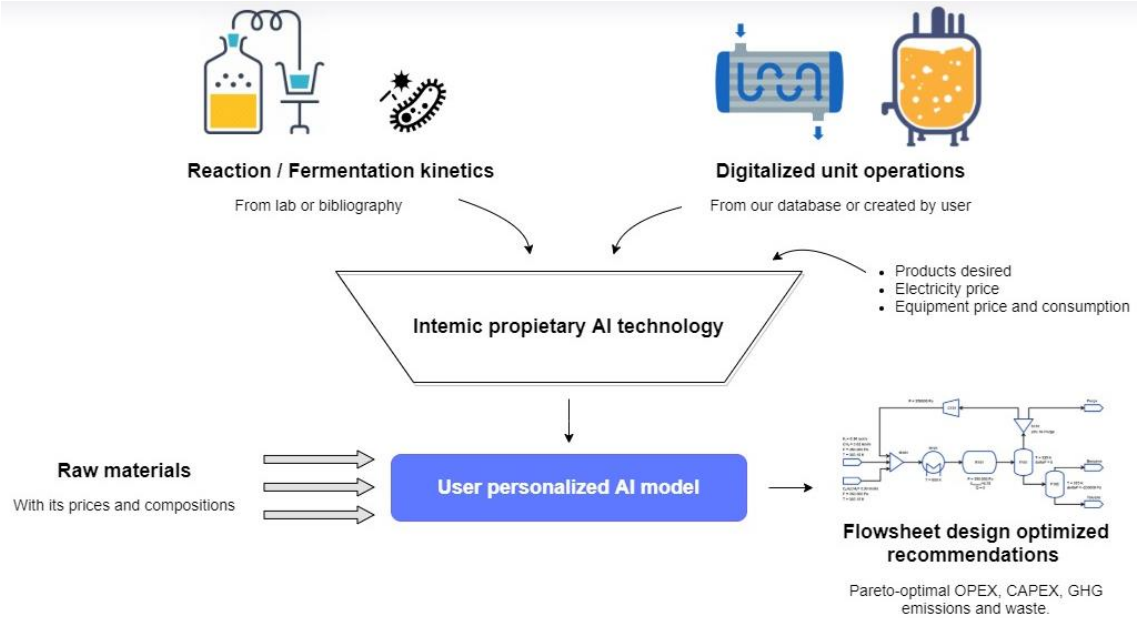


Figure 4. *Flowsheet Copilot is the software built by Intemic that automates the techno-economic and the life cycle assessment of new biorefineries by using RL*

Why is it especially good for biorefineries?

Once the AI model explored the space and its properly trained, it can generalize for different feed compositions, generating optimized flowsheets in real time, which is interesting in biorefineries or waste valorization where feed composition can vary easily because of its type or different location. Also, because of the high number of streams that a biorefinery can have, a lot of costs in CAPEX and OPEX can be saved thanks to an intelligent flowsheet design, using energy and raw materials intelligently thanks to the long-term strategies

One of the features that makes reinforcement learning a powerful tool is that it can give real time updated recommendations in each step of the design, as a copilot, while the engineer can take the decisions. This approach combines the engineer intuition with the AI knowledge generated by the previous realization of millions of simulations.

About the autor:

Albert is the Founder and CEO of Intemic, a software company that builds digital solutions for the process industry, by combining the latest techniques in AI with process engineering.