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Towards White-box Environmental and Economic Process Optimization: Tailoring Modelling Approaches to Multi-scale Simulations.

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ABSTRACT

Polylactic acid (PLA) is the most produced bioplastic, however, for it to compete with fossil-based plastics, maximum production efficiency is crucial. To achieve this, all scales, from catalyst scale to process scale, must be simultaneously considered. This challenge is particularly relevant for PLA production, where complex interactions of multiple phenomena occur in several unit operations and the development of active non-toxic catalysts is of major importance. For these reasons, developing a framework that allows a comprehensive understanding of the influence of design choices at different levels is of paramount importance. To address this, a multi-scale model was developed for the PLA production, coupling a custom devolatilizer reactor model to a process simulator that is subsequently linked to an environmental assessment tool via Python-based interfaces. With this model, sensitivity analysis was performed to assess the influence of operational variables on the most relevant KPI's. Results showed that changes of only 5.5 torr in the devolatilizer pressure can lead to total utility consumption and climate change impact variations of 13% and 2%, respectively. This demonstrates the critical role of the devolatilizers in the process, highlighting the importance of developing custom unit operation models coupled to the process simulator. Additionally, the results show that, with this framework, the influence of reactor scale variables on industrial environmental performance can be seamlessly assessed. Overall, this work demonstrates the feasibility and value of integrated multi-scale modeling for sustainable process design and provides a solid foundation for the future development of a multi-scale environmental and economic optimization framework.

Keywords: Sustainable process design, Multi-scale modeling, Custom unit operation model, Automated environmental assessment

INTRODUCTION

Polylactic acid (PLA) is the most produced bioplastic [1], but its carbon footprint, among other environmental metrics, still has margins that need to be improved, together with the production cost. To achieve utmost efficiency, all scales matter, from phenomena in a given unit operation to mass and energy integration, making multi-scale models necessary for the optimization of these processes. Currently, as the design of sustainable processes is mostly performed independently at different scales, the overall influence of design choices at different levels is not assessed in a seamless way, leading to a trial-and-error and inefficient design workflow.

In particular, in the case of PLA production, there are intricate interplay of mass-transfer, evaporation, and reaction phenomena in several unit operations [2]. Additionally, at the moment, stannous octanoate (tin octanoate, $Sn(Oct)_2$), is commonly used as a catalyst. Although classified as food safe, toxic tin can be released in the environment during PLA degradation [3]. Therefore, ongoing research is being made to develop nontoxic metal-based catalysts for this process [3]. To efficiently evaluate the impact of using different catalysts on the overall economic and environmental performance of the process, a multi-scale model is essential.

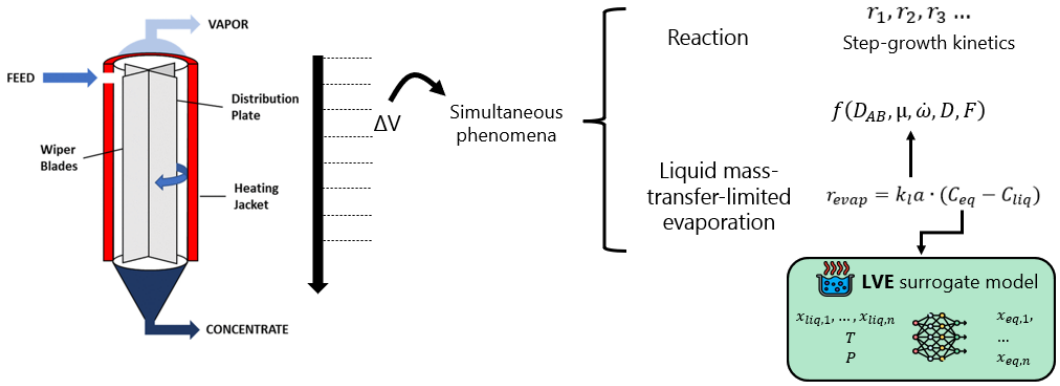

Figure 1. Schematic of the devolatilizer [6] used in the depolimerization reaction and the final PLA purification as well as a schematic for the custom reactor model developed.

To address this topic, in this work, a multi-scale model for PLA production was developed. As of today, the model covers the reactor, process, and environmental analysis scale. The process scale is simulated in Aspen Plus, to which a custom devolatilizer model is coupled using the Python Unit Operation tool [4].

For the environmental analysis, a Python interface that links the process model with OpenLCA is used. With this multi-scale model, sensitivity analysis was performed to evaluate the impact of different possible decision variables on relevant technical and environmental KPI's. The knowledge gained in this paper is crucial for the future development of a holistic optimization algorithm.

METHODOLOGY

Reactor-scale model via Python-implemented detailed devolatilizer model

The synthesis of PLA, starting from lactic acid, consists of three steps: oligomerization of lactic acid into a PLA pre-polymer with low molecular weight (MW ~1 kg/mol), depolymerization into lactide, and ring-opening polymerization (ROP) into high molecular weight PLA (100 kg/mol). In the depolymerization reaction, the low molecular weight PLA, with the aid of the catalyst, converts into lactide. However, if the lactide remains in the reaction mixture, the reaction will reach an equilibrium at low pre-polymer conversions. To favor the product side of the reaction, the lactide must be continuously removed from the liquid reaction mixture into the vapor phase. As the reactional mixture is quite viscous, due to the pre-polymer's molecular weight, the mass-transfer of the volatile components (water, lactic acid and lactide) from the liquid mixture to the liquid-vapor interface is limited, rendering the evaporation of the product and thus the progression of the reaction quite challenging. In the final high molecular weight PLA mixture purification, the viscosity of the mixture is even more relevant, turning the evaporation of the volatiles even more mass-transfer limited. For these reasons, in industry, both the depolymerization and the final PLA purification are performed in depolymerization equipments [5], schematized in Figure 1.

In these equipments, the liquid polymeric feed mixture travels in a thin liquid film, forced by the movement of wiper blades, reason why the equipment is also called "wiped-film evaporator". Being the mixture in a thin film, the liquid-vapor interfacial area is maximized, necessary to counteract the mass-transfer limitations in the liquid phase. This way, with high temperatures being maintained with heated jackets, the volatile components, such as lactide, will evaporate and leave the reactor in the vapor phase at the top of the equipment, while the polymeric mixture will leave the reactor at the bottom of the equipment. As Aspen Plus lacks a built-in model to adequately simulate all phenomena (reaction, mass transfer and evaporation) simultaneously, a custom model was developed to simulate the devolatilizers. The models were developed using the Python Unit Operation (PUO) [4], a CAPE-OPEN complying tool, that allows integration of Python code into process simulators, as can be seen in Figure 3, in which the devolatilizer models are identified as "*Python Unit Operation*" boxes.

As schematized in Figure 1, the reactor model discretizes the reactor volume into several control volumes. In each control volume, the reaction rates are calculated via step-growth kinetics implemented from literature [7]. Then, the evaporation rates of each component, $r_{evap,i}$, are computed using Equation 1, where $k_{l,i}$ is the mass-transfer coefficient of component *i* in the polymeric mixture, a is the interfacial area, $C_{eq,i}$ is the equilibrium concentration in the liquid phase, and $C_{liq,i}$ is the liquid phase concentration of component *i*.

$$r_{evap,i} = k_{l,i} a \bullet (C_{eq,i} - C_{liq,i}) \quad (1)$$

The mass transfer coefficient in devolatilizers is calculated through several thermodynamic and fluid mechanic correlations from literature [8] and will depend of a number of different variables, such as the diffusivity of the volatile components in the in the polymeric mixtures (estimated with Stokes-Einstein equation), D_{AB}, the viscosity of the polymeric mixture, μ, the rotation speed of the wiper blades, $\dot{\omega}$, the diameter of the equipment, D, and the flowrate of the liquid mixture, F. The viscosity of the polymeric mixture is calculated as a function of the solute weight fraction, the molecular weight of the polymer, the temperature and the shear rate proportioned by the wiper blades through correlations given in the literature [9].

For the liquid-vapor equilibrium (LVE) concentrations calculation, a PUO-integrated function that connects to the process simulators thermodynamic model exists, however, as this would have to be done in every control volume, it would lead to high simulation times (up to 1 hour for a single run) and convergence issues that would render a future optimization framework very inefficient. Instead, neural networks (NN) were trained on the PolyNRTL thermodynamic data to calculate the LVE compositions at every control volume of the reactor. The NN model inputs are the input compositions, temperature, pressure, and molecular weight of the polymer, and the output data are the liquid-phase output compositions at equilibrium. In Figure 2, the parity plot for the testing of the NN used to calculate the lactide liquid equilibrium compositions with a 5% error cone is presented. In this case, the NN has 3 layers with 20, 16 and 12 nodes.

Process-scale model

This process model focuses on the transformation of lactic acid to PLA, as licensed by NatureWorks [5] (the largest PLA producer globally), based on an earlier implementation [7]. The simulations were done in Aspen Plus v14 software using its Polymer Plus module and PolyNRTL as thermodynamic method [7]. The process has three steps (see Figure 3): oligomerization of lactic acid into pre-polymer, its depolymerization into lactide, and, after a purification step, the ROP reaction into PLA, followed by the purification of the final PLA product. By default, detailed models were selected from the Aspen library apart from the devolatilizers, as mentioned previously.

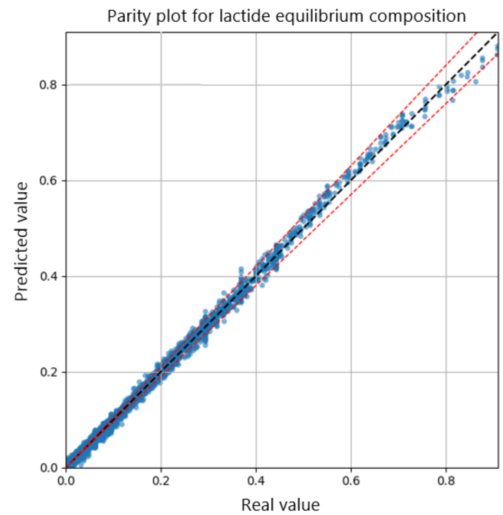

Figure 2. Parity plot of the neural network trained to calculate the lactide equilibrium liquid composition. The neural network uses 3 layers with 20, 16 and 12 nodes.

For the oligomerization step, lactic acid is converted into pre-polymer in a stirred-tank reactor connected to a distillation column to remove the produced water. The base case operating conditions of the reactor are 172°C and 400 torr [7]. Next, the pre-polymer is depolymerized in a devolatilizer, i.e., an agitated thin-film evaporator, with simultaneous removal of volatiles, which will be further explained in the next section. The base case conditions for the reactor are an inlet temperature of 170°C and an outlet temperature of 210°C at 5 torr [7]. The non-reacted pre-polymer is recirculated into the reactor, while

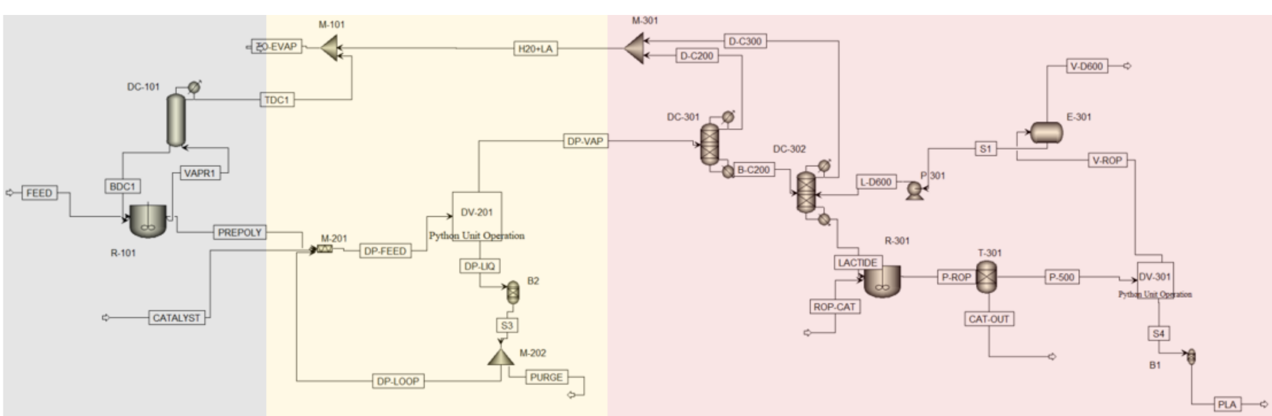

Figure 3. Aspen Plus model flowsheet developed in this work for the production process of PLA divided into three sections: Oligomerization in grey, depolymerization in yellow and ring-opening polymerization in red.

the produced lactide stream continues to the ROP section. This section starts with a purification section, constituted by two distillation columns. In the first column, the water from the lactide mixture is removed, while in the second column, the lactic acid is removed, both in the distillate, to render a purified lactide mixture in the base of the second column. The lactide stream is then converted, in a second stirred-tank reactor, into high MW PLA which undergoes a final purification in a devolatilizer to remove impurities. At the base case, the stirred tank reactor operates at 170ºC and 1 atm while the devolatilizer operates at 180ºC at the inlet, 200ºC at the outlet and 0.5 torr [7]. The crystallization process to form the PLA pellets was not simulated in this work.

To ensure that the modeled process produces the desired PLA production in terms of flowrate, molecular weight and purity, design specs were added to the Aspen Plus simulation. To fix the PLA flowrate at 8610 kg/hr (estimated value for a single production line of PLA), the lactic-acid feed mixture (88% wt.) flowrate is varied. The molecular weight of 100 kg/mol is ensured by varying the DC302 column distillate flowrate, as the molecular weight of the PLA produced will be mainly controlled by the purity of the lactide mixture that enters the ROP reactor. The higher the purity, the higher the molecular weight of the produced PLA will be. Finally, the purity of the final PLA mixture was kept at 98% wt. by varying the length of the DV301 devolatilizer, which can be translated into the number of devolatilizers needed in series. The values of the main KPI's for the base case operational variables values can be found in Table 1.

LCA model via Python interface

To perform an accurate and holistic environmental assessment of the modeled process, OpenLCA, an open-source LCA tool, was used. The LCA analysis was done with "*cradle-to-gate*" borders, meaning that the environmental impact includes the impact of all production processes from the extraction of the raw material up to the PLA product leaving the factory gate. This LCA analysis excludes the impact of the use of PLA and of its end-of-life. The Ecoinvent 3.11 was used as a database for the LCA analysis. The CML v4.8 2016 impact assessment method was used in the work. The LCA model consists of adding up the environmental impact of the necessary lactic acid production, for which the environmental impact was already defined in the database (corresponding to the production process of the manufacturer Cargill) and the environmental impact of the production of the different utilities used in the transformation of the lactic acid to PLA (such as steam, electricity and water). The climate change impact of 1 kg of lactic acid, through the Cargill production process, is 4.50 kg CO_2 eq.

To perform the LCA analysis, the necessary parameters to extract from the Aspen Plus process model are the lactic acid flowrate and the different utility usages. To extract these values, a Windows COM automation interface between Aspen Plus and Python was developed using the *win32com* library and Aspen's Variable Node Tree structure. Using this interface, the values from Aspen's simulation can be extracted, new parameter values can be set and new simulations can be run, which is critical for the sensitivity analysis performed in this work, and the future optimization framework. To run the LCA model with the values extracted, the *olca* library was used, which allows the coupling of the Python script with the OpenLCA model.

RESULTS AND DISCUSSION

Before implementing an optimization framework, it is crucial to identify the operational variables that influence the KPI's to be optimized, as these are best suited to be the decision variables. The operational variables tested were the ones related to the most relevant equipment. This leads to the following variables: the temperature and pressure of the reactors R101 and R301 and of the devolatilizers DV201 and DV301, and the blade rotation speeds of DV201 and DV301. Additionally, the influence of the length (proportional to the number of equipment in series) of DV201 will also be analyzed.

With the goal of understanding the impact on the process as a whole, KPIs from a technical, economic and environmental point of view will be selected. From the technical side, the process yield (PLA production flowrate divided by the lactic acid feed flowrate) will be analyzed. As the product flowrate is fixed by a design spec, in practice, variations in the process yield describe variations in the lactic acid feed flowrate. From the economic side, as a complete techno-economic analysis has not yet been implemented, the operational costs can be related to the necessary feed flowrate (already analysed by the process yield) and the total utility consumption, which will be used as a KPI. Regarding capital costs, its variations in these sensitivity analyses will only be due to changes in the necessary DV301 length necessary to obtain the desired PLA purity. For this reason, the DV301 length will be another KPI tracked. Finally, to assess the variations in environmental impact, the changes in the climate change impact will be analyzed, although with the developed LCA coupling, the influence on any other environmental KPI could also be analyzed.

The KPI values obtained for the base case operating conditions will first be presented, followed by the qualitative influence of each operating variable on the KPIs. Then, the main variables impacting each KPI will be discussed in more detail.

Base case results

At the base case, corresponding to the operating

Table 2: Influence of different operational variables ("T" – temperature, "P" – pressure, "$\dot{\omega}$" – blade rotation speed) on technical and environmental KPI's. Squares filled in green (or with "++") indicate strong influence of the variable on the KPI, yellow (or "+") indicate some or weak influence, red (or "0") indicate irrelevant or no influence and grey indicate variables that can't be changed or for which the simulation doesn't converge.

	Process yield			Total utility consumption		
	T	P	$\dot{\omega}$	T	P	$\dot{\omega}$
R101		+			+	
DV201	+	+	+	+	++	+
R301	0	0		+	0	
DV301	0	0	0	+	+	+
	DV301 length			**Climate change impact**		
	T	P	$\dot{\omega}$	T	P	$\dot{\omega}$
R101		++			+	
DV201	0	++	+	+	+	0
R301	+	0		0	0	
DV301	++	++	++	0	+	0

conditions mentioned in the process scale section, we obtain the following KPI values, presented in Table 1.

Table 1: KPI values obtained for the base case scenario.

KPI	Value
Process yield	64.52 %
Total utility consumption	13.91 MW
DV301 length	84.12 m
Climate change impact	6.869 kg CO_2 eq/kg PLA

The normalized utility consumption is equal to 5.82 MJ/kg PLA. Regarding the DV301 necessary length, it is considered that the devolatilizers have a maximum length of 6 meters and that all devolatilizers are placed in series (in order for the residence time to be inside the recommended operating range). This implies that 84.12 m is equivalent to having at least 14 devolatilizers in series. The number of devolatilizers, in both the case of the DV301 and the DV201, seems to be excessively high. This might be due to low diffusivity values calculated for the volatile components in the liquid mixture, which, for now, are calculated using the Stokes-Einstein equation. Future efforts will be made to obtain more accurate diffusivity values for this system, which will likely decrease the number of devolatilizer equipments necessary. Nonetheless, it has been noted that once the process is optimized, the number of necessary devolatilizers will be decreased significantly.

Impact on process yield

In Table 2, the impact of the different operating variables on the KPI's mentioned can be observed. Regarding the process yield, the most influential operational variables are related to the R101 and DV201 reactors, which is natural as these are the equipment
more upstream of the process, having more influence on the overall process than the more downstream equipment. For instance, increasing the operating temperature of DV201 to 175°C increases the process yield to 64.96%, as it promotes a more effective product evaporation from the reactional mixture. The increase in the process yield is equivalent to the decrease in the necessary feed flowrate, which drops from 13340 to 13252 kg/hr.

Impact on total utility consumption

When it comes to total utility consumption, more operational variables have an impact. The most notable impact is noted with the DV-201 pressure. With lower pressure, such as 2 torr, the total consumption decreases to 13.24 MW, while at higher pressures, such as 7.5 torr, the total consumption increases to 15.25 MW. These relations are likely described by the increase and decrease in the process efficiency, which overcome the increase and decrease in vacuum costs, respectively, as lower pressures favor a more efficient lactide removal.

Impact on necessary DV301 length

Regarding the impact on the necessary DV301 length, which translates into the number of devolatilizers in series and is naturally related to the necessary capital investment cost, it is intuitive that the variables related to the same equipment have a more significant impact. In Figure 4, it can be seen that at higher DV301 inlet temperature, the necessary length decreases significantly. For a temperature of 187ºC, the necessary length is less than 60 m, corresponding to 10 devolatizers. In the same way, in Figure 5, it is seen that higher rotation speeds lead to lower lengths, with rotations of 250 rpm leading to a length of 74 m. Both relations are expected as the increase in both variables favor a more efficient volatile evaporation from the polymeric mixture, as increased rotations increase the mass transfer coefficient of the volatile components.

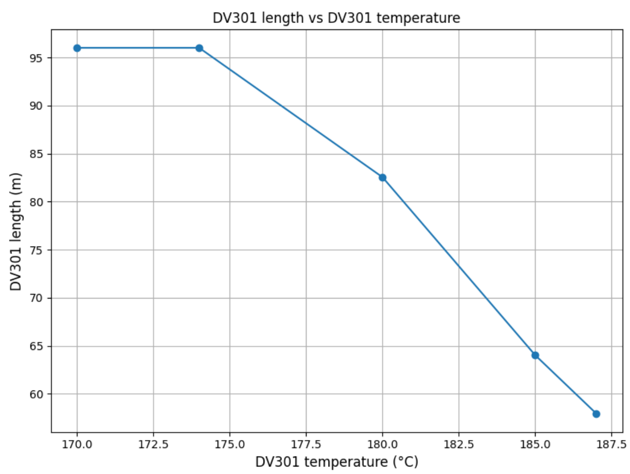

Figure 4. Impact of the DV301 temperature on the necessary DV301 length to perform the desired purification of the final PLA product.

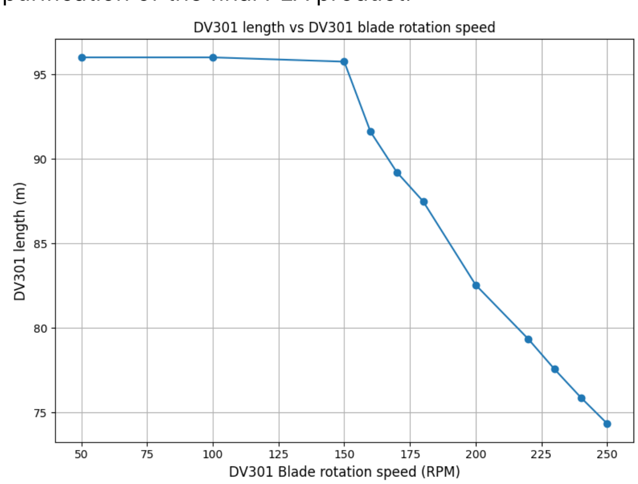

Figure 5. Impact of the DV301 blade rotation speed on the necessary DV301 length to perform the desired purification of the final PLA product.

Impact on climate change impact

In the case of climate change impact, in general, the more impactful variables are the ones that impact the feed flowrate and the energy consumption, as these are the main contributors to the environmental impact. For instance, the DV201 pressure has an influence on both the feed flowrate and the energy consumption, so naturally, as can be seen in Figure 6, it also has an influence on climate change impact. The influence is, however, not very significant, with the climate change impact decreasing to around 6.81 kg CO_2/kg PLA at 2 torr and increasing to 6.95 kg CO_2/kg PLA at 7.5 torr.

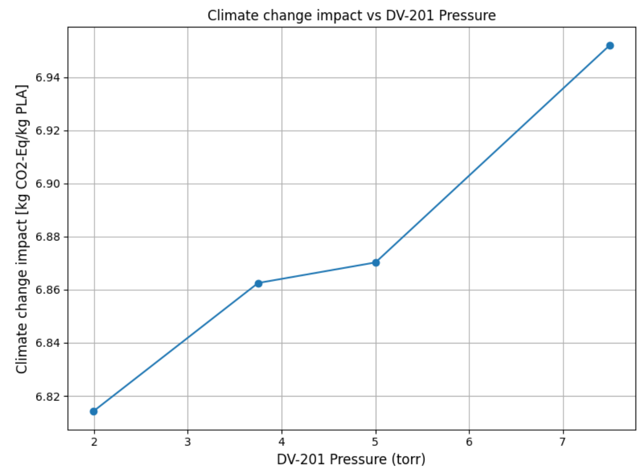

Figure 6. Impact of the DV201 pressure on the overall climate change impact.

In the case of the devolatilizers DV201 and DV301, variables such as temperature, pressure and blade rotation speed are all reactor-scale specific, as their impact couldn't be captured (at least not fully) without the custom devolatizer models developed. Thus, in Figure 6, we see the impact of a reactor scale variable directly on the environmental impact and in Figures 4 and 5 the impact, indirectly, on the capital investment cost. This is only possible with the coupling of the reactor, process, and environmental analysis scales as presented in this work.

DV201 length influence

In addition to the potential decision variables presented in Table 2, the impact of the length of DV201 (which in practice can be translated into devolatilizers in series) was analyzed. In the base case scenario, a length of 90 meters is used, which translates to 15 devolatilizers in series in two parallel production lines (in order to be inside the recommended residence time range), making a total of 30 devolatilizers. For the sensitivity analysis, the length was varied between 60 and 114 meters (20 and 38 devolatizers). The impact on the different KPI's can be seen in Table 3.

Table 3: Impact of the DV201 length on the different KPI's analyzed.

KPI	KPI Value for respective DV201 length 60 m	114 m
Process yield (%)	63.77	64.89
Total utility consumption (MW)	12.63	13.86
DV301 length (m)	96.00	83.19
Climate change impact (kg CO_2 eq/kg PLA)	6.875	6.831

As seen in Table 3, the DV201 length has an impact on all KPI's. Higher DV201 lengths favor lead to higher conversions, leading to more favorable KPI values. However, higher DV201 lengths also lead to higher capital cost investment and higher total utility consumption. This leads to an interesting trade-off between different KPI's, which could be explored in more detail with a future optimization framework.

The variables with the most significant impacts on the KPI's are the ones that should be chosen to be decision variables in an optimization framework. Having in account the analyses done, we conclude that the most important decision variables to include in an optimization framework are the following ones (in descending order): DV201 pressure, R101 pressure, DV201 temperature and blade rotation speed, DV301 pressure, temperature, and blade rotation speed, and finally, R301 temperature. Once the convergence of the process simulation is improved, the influence of the R101 temperature on the KPI's should be analyzed in more detail.

CONCLUSIONS AND FUTURE WORK

The first outcome of this work is how it shows the possibility of integrating models of different scales in a seamless manner and only using open-access tools. With the Python Unit Operation tool presented in this work, any complex unit operation at a smaller scale can be modeled in Python and coupled to a wide variety of process simulators (including Aspen Plus). Using a Python interface and the *olca* library, LCA analysis using OpenLCA can be performed, as long as the process simulator can be linked to a Python interface, which is the case with Aspen Plus.

With the sensitivity analysis performed, it was concluded that the variables related to DV201 and the temperature of R101 have a significant influence on practically all the KPIs considered, being the most relevant variables to be used in a future optimization algorithm as decision variables. The exception is the necessary DV301 length, for which the variables related to the DV301 devolatilizer have the largest influence. The crucial importance of both devolatilizers in the process highlights the paramount importance of having developed and coupled the detailed devolatilizer model, in order to understand the full influence of the devolatilizers on all KPI's with precision. With this coupling of the models, we were able to solve the common problem of assessing the impact of decision variables at smaller scales on industrially relevant environmental and, eventually, economic KPIs in an effortless way.

Future work will address, firstly, on improving the robustness and stability of the multi-scale model, so that the influence of all operational variables can be assessed at their full operational range. Additionally, future work will focus on coupling a complete techno-economic analysis tool in the same Python interface already used for the LCA analysis, so that the process can be accurately assessed not only environmentally, but also economically. Finally, the optimization algorithm can be developed in the Python interface, creating a multi-scale optimization framework, with which variables at all scales, potentially even catalyst-scale, can be optimized to improve the industrial economic and environmental performance of PLA production.

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