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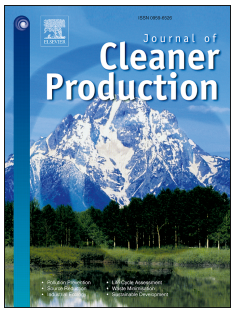

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A decision-support framework for techno-economic-sustainability assessment of resource recovery alternatives

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Abstract

The careful consideration of technology readiness, economics and sustainability holds the key to identifying and then transitioning a resource recovery opportunity into actual implemented solution. Currently this decision-making process is carried out based on in-house experience of stake-holders as there is no established framework that can be followed. This work presents a systematic computer-aided decision-support framework to tackle challenges faced when attempting to identify and develop resource recovery projects. The framework is hierarchical and combines key evaluation aspects in one integrated approach. The framework will enable industries transition towards more sustainable production, providing users with the opportunity to evaluate and support decisions on not only a financial basis, but also from a comprehensive techno-economic and sustainability angle. To this end, the framework collects relevant aspects within the sustainability field and addresses concepts such as circular economy, resource recovery, and waste management. This research also aims to add additional relevant inputs for increasing the possibilities to reach the scope of cleaner production. The proposed methodology is generic and can be applied to a wide variety of potential resource recovery projects. The application of the framework is highlighted through an industrial case study of the monosaccharide recovery from wheat straw liquor in bio-refinery setting.

Keywords

Resource Recovery, Circular Economy, Commercialisation, Technology, Environment, Techno-Economics

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1. Introduction

For more than 200 years the world economy has followed a linear economy model of 'take-make-dispose' [1] where resources are extracted for producing goods and then discarded as waste. In this model economic value is created by maximizing production [2] and has created large consumer markets in the past decades [3]. In the last few years, circular economy has been receiving increasing worldwide attention as a way to overcome the linear economy model [4,5]. Recovery of resources from waste streams is one type of approach that can lead to circular economy. As summarized in Figure 1, resource recovery acts as a key platform approach to close the loop of several production processes, giving the possibility to obtain valuable products that can be used as raw materials for the same process, or sold as new products. This allows companies to achieve the goal of sustainable production and consumption, improving their product portfolio.

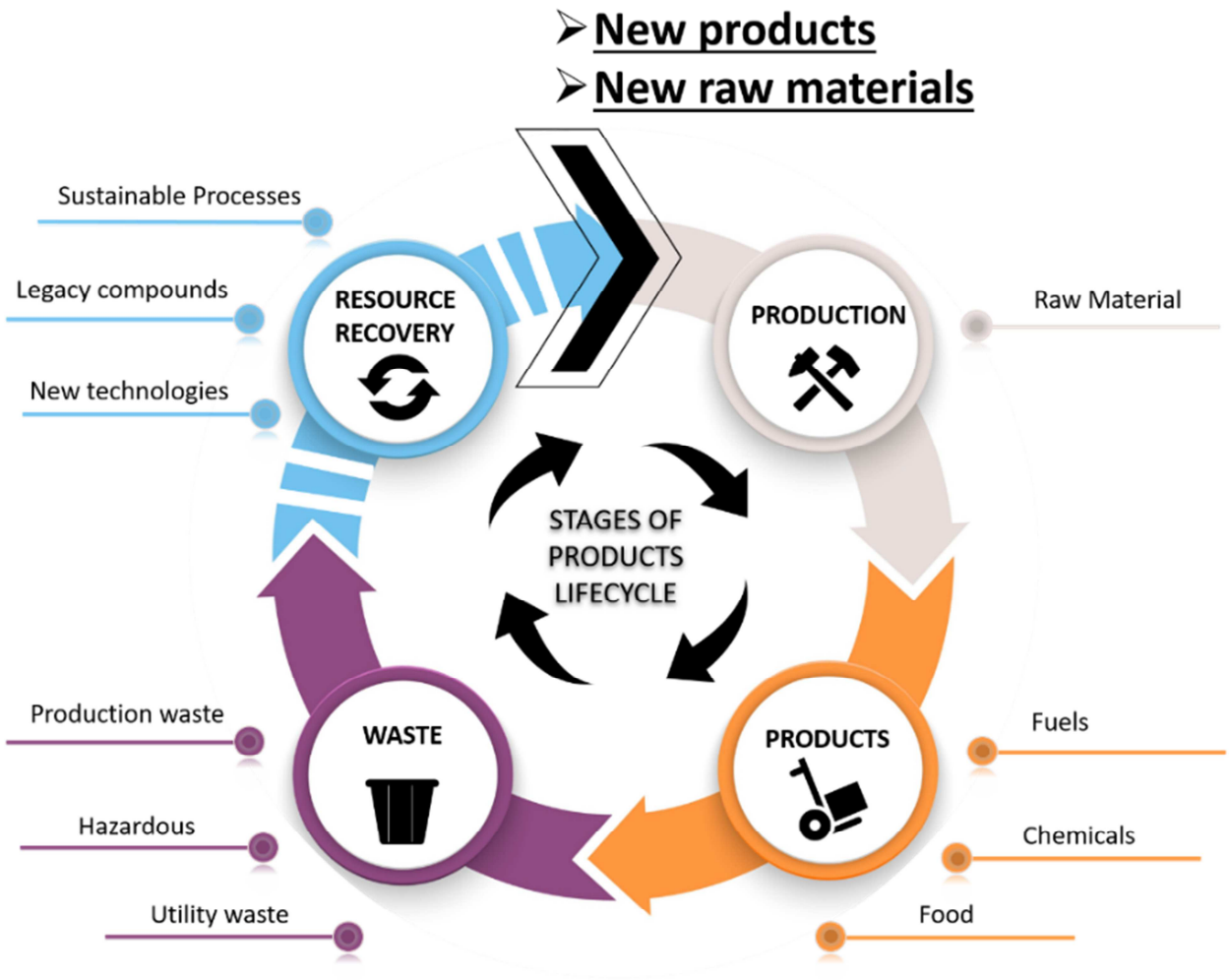

Figure 1: Resource recovery as the closing element to reach the goal of circular economy for products lifecycles.

Currently, the use of resource recovery finds good expression in many different industrial processes, among which the industrial applications related to the dairy industry [6] and biodiesel by-products production[7]. In petrochemical operations, waste reintegration is also practiced widely [8]. Unfortunately, recycling and reuse can be sometime hampered by the presence of certain chemicals which constitute technical barriers to resource recovery [9] [10]. These substances are usually hazardous compounds to both humans and the environment and they constitute one of the main obstacles to circular economy. All these substances, called 'legacy compounds' derive from incidental contamination throughout the product lifecycle, as well as from the fact that new chemicals are continuously placed on the market whilst others are forbidden due to environmental risks. These compounds have a potential to be high value-added compounds and therefore worth of being considered under the aspect of resource recovery [10].

Looking at a particular example, as it can be the bio-based industry, from the state of the art it emerges that the underutilized waste streams of bio-based production processes offer great potential in the field of resource recovery [8]. From a holistic perspective, bio-based industry are relatively immature and initially encounter resource abundance, thus perceived little demand for reuse of potentially valuable recoverable compounds [11,12].

Resource recovery is an area with many different facets. It has a dynamic nature for which it is multiscale and multidimensional. With the adjective multiscale, it is defined a problem that starts at small scale and generates consequences on large scale. On the other hand, multidimensional stands for the accounting of many different aspects at the same time such as technological, environmental, social and economic ones. However, to the best of the author knowledge there is no integrated single solution that can be used in tackling these facets. For example in the previous works [8,11–14] where a system's thinking approach was used to tackle some of these facets are considered from an overall analysis point of view. The main focus of this work is on the development of a tool that can be used as a starting point to addressing the problems that revolve around the waste stream management sector, and resource recovery opportunity, in a more systematic and efficient way. Therefore, it aims at proposing an approach that can facilitate the early-stage decision-making process for exploring resource recovery opportunities.

At the early stage of the decision process, and in order to mitigate waste, we need a method to identify resource recovery opportunities. The systematic decision support framework proposed in this work aims at suggesting solutions that can be further evaluated. With this tool, we foresee the possibility to overcome several limitations related to economic, technical and environmental aspects. In fact, this paper proposes a new economic outlook that considers all the technical, economic, and environmental issues in a more uniform and systematic way.

2. Framework

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The framework can be compartmentalized into five segments, each defined by a characteristic question. The user must provide the required inputs and perform the associated algorithms to answer these questions and progress through the framework. Throughout the framework, additional questions are posed in the form of decision gates, aiming to govern and control a user's progression through the process. An overview of the framework is presented in Figure 2. As it can be seen, it is divided into four layers of decision making, (1) Potential identification, (2) Separation technology selection, (3) Feasibility assessment, (4) Techno-economic evaluation. The framework has a gated decision-making structure which allows each step to be used independently depending on the specific problem to be solved.

- What is the objective of resource recovery implementation?
- Is there economic/environmental potential in recovery?
- What are the most thermodynamically feasible separation pathways?
- Are the separation pathways physically/economically feasible?
- Are the separation pathways sustainable?
- Is investment justified?

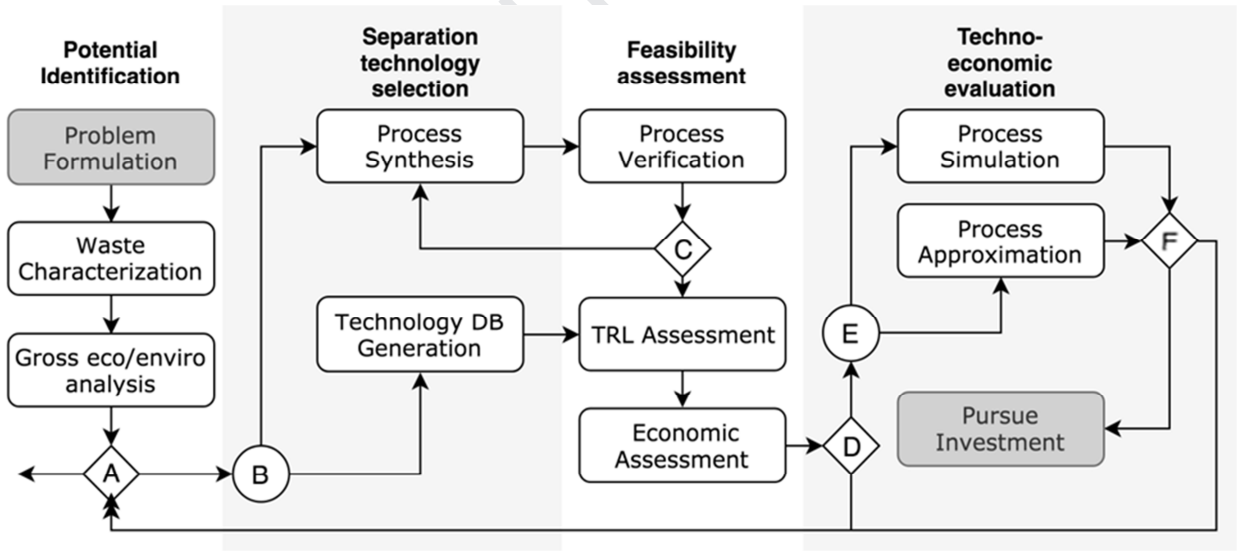

Figure 2: Schematic representation of the workflow of the methodology. Grey framework steps indicate input/output.

2.1 Interval 1: Potential Identification

2.1.1 Problem Formulation

The first and most instrumental task of framework construction is the problem formulation. It is here that the aim, objectives, and scope of the design problem are outlined mathematically. The objective function is

formulated to fit an agenda, and demonstrates the desired outcome of the design problem. The success of the process solution will be a result of direct satisfaction of the objective function.

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Algorithm 1.1: Problem formulation

Objective: Formulate objective function

Step (i): Record information pertinent to the objectives and motivations of the resource recovery potential identification process being applied.

Step (ii): Identify the metric(s) that must be maximized to reach the objective and apply them to the generic template function.

$$\max f(x)$$

If there are any constraints present, identify them in the following manner:

$$subject\ to. \qquad h(x) = 0, \qquad g(x) \leq 0, \qquad x_{min} \leq x \leq x_{max}$$

2.1.2 Waste characterisation

The process stream to be studied must be characterized. Therefore, the user builds a comprehensive understanding of the stream composition and relevant properties, providing a strong basis for framework data collection. Thus, Algorithm 1.2 is applied.

Algorithm 1.2: Target stream characterization

Objective: Obtain relevant cases for future assessment

Step (i): Determine stream composition, record components of significant concentration either by experiments or from literature. Assign numeric indicators to the components, $1,2,\ldots,NC$. These indicators are used to reference property values to the components they represent.

Step (ii): Perform a literature search on the obtained components to determine if they are commonly reacted to create products, removed due to inhibiting characteristics, or lumped to

form pseudo-components. Update NC, and assign numeric indicators to the newly included pseudo-components and products, if any.

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Step (iii): Generate case 1, from the stream components, $c = 1$.

Step (iv): If no reactants or inhibitors are present, number of cases is equal to one. Elsewise, generate all possible scenarios from the information gathered in step (ii), and record them as different cases. Assign each case a numerical value and generate a vector of cases, set the final number of cases equal to n: $c_1, c_2, \dots, c_n$.

2.1.3 Gross sustainability potential

Once the problem has been formulated and stream characterized, steps can be taken to reduce the number of candidates available in the search space. The proposed methodology assesses the stream from economic and environmental perspectives with the intention of identifying target compounds.

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Algorithm 1.3: Gross sustainability potential and environmental impact overview

Objective: Obtain gross sustainability potential and environmental impact

Step (i): Specify component concentration, C_i, molar mass, MW_i, stoichiometric coefficients, a_i, b_i, c_i, market value, pp_i, cost to remove one kilogram of COD, tc , and is the social price of carbon, cc.

. For pseudo-components take the summation of their constituent's properties. For reaction products, determine concentration with reaction stoichiometry.

Step (ii): Apply the stoichiometric carbon and treatment cost methodology explained to determine economic parameters for the components of case c.

Note: If inorganic resort to literature search to obtain the information required.

Perform the following $for\ i = 1,2,\dots,NC$. COD_i and CO_{2_i} refer to the theoretical chemical oxygen demand of component i and the the carbon equivalent of component i.

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$$(C_aH_bO_c)_i + X_i^1 \cdot O_2 \rightarrow X_i^2 \cdot CO_2 + X_i^3 \cdot H_2O$$

$$\begin{bmatrix} C \\ H \\ O \end{bmatrix}_i : \begin{bmatrix} a \\ b \\ c \end{bmatrix}_i^s + X_i^1 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} = X_i^2 \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} + X_i^3 \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}$$

$$X_i^2 = a_i^s\,, \qquad X_i^3 = \frac{b_i^s}{2}\,, \qquad X_i^1 = \frac{X_i^3 + 2X_i^2 - c_i^s}{2}$$

$$COD_i = \frac{C_i}{MW_i} \cdot X_i^1 \cdot MW_{O_2}\,, \qquad CO_{2_i} = \frac{C_i}{MW_i} \cdot X_i^2 \cdot MW_{CO_2}$$

Step (iii): Determine gross economic sustainability potential value, $for\ i = 1,2,\dots,NC$. Where P_i, Tc_i, and CC_i are the total value, current treatment, and social cost of carbon factors.

$$P_i = pp_i \cdot C_i\,, \qquad Tc_i = COD_i \cdot tc\,, \qquad CC_i = CO_{2_i} \cdot cc$$

$$GSP_i = P_i + Tc_i + CC_i$$

Note: If a reaction occurs, assess if the reactants are easily recoverable, or pertain value at low purity. If this is the case, deduct the reactants value from the products.

<u>Decision gate A</u>

Check if any of the components satisfy the threshold gross economic sustainability potential, $Threshold$ set in the problem formulation framework step. Set the component with the largest potential as the target component.

$$if\ GSP_i > Threshold : Target = V_i,\ \ for\ i = 1,2,\dots,NC$$

Note: It is possible to assign two target components if two values share similar promise.

Remark: If the minimum threshold is not met, financially motivated resource recovery is not feasible in this context, exit the framework.

Remark: If downstream decision gates D or F reject the set target compound, iterate back to this step and assign the next most promising component as the target for recovery.

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2.2 Layer 2: Separation Technology Selection

In this section of the framework viable separation technologies for the recovery of the stream constituents are identified. Such technologies can then be sequenced to provide a physical feasible process synthesis for the recovery of the afore-determined target components, thus answering the associated characteristic question. The complexity of the stream composition affects the downstream processes significantly and is evaluated prior to beginning the section. The separation schemes of streams of binary or ternary compositions should be furnished via literature search, whereas more complex compositions should be subject to process synthesis techniques.

Option gate B

Option gates differ from decision gates in their discreteness. Whilst decision gates are binary and must be one or the other, option gates provide two applicable options, splitting the pathway. The purpose of the option gate is to guide the user to select the framework pathway that best suits their case. However, if no suitable solution is generated from this route, the user may revert back to the option gate and select the other framework pathway before eliminating the component from contention.

Separation task flowsheets should be furnished by process synthesis techniques where applicable (algorithm 2.2), with the remainder subjected to technology database generation and manual pairing (algorithm 2.1). Algorithm 2.2 may also be favourable in instances that substantial information is known about the case studied, or that the case is a binary or ternary system.

2.2.1 Technology database generation

In instances where the system is not very complex, furnishing the process flowsheet manually may be preferred. Literature searches including a patent search are undertaken to identifying physically and technically feasible separation operations by systematically taking into consideration the class of separation methods as well as the properties of the mixture to be separated. In this context a physically capable separation technology refers to a technology that is capable of separating the desired compounds (i.e if the

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relative volatility between two components is the same, then thermal separation is not physically feasible. The resultant pathway is the translated into a pre-defined data structure so that it can progress through the framework.

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Algorithm 2.1: Technology database generation

Objective: Obtain technically feasible flowsheet

Step (i): Perform a literature search on systems containing similar components and processes to provide a basis for technology screening.

Step (ii): By starting from the least complex potential separation task solution, begin the screening process. In this instance a simple separation task is defined as a task where there is a high driving force difference for a given separation technology. Such as use of distillation (thermal separation) for a separation task with a large relative volatility difference. After physical and technical feasibility is addressed, the screening must first be governed by the objective function and the accompanying constraints.

Remark: If more than one candidate remains apply tertiary constraints, until as singular option emerges. For example a constraint related to temperature sensitivity of the mixture. In this instance, if separation can be performed by both thermal distillation (thermal separation) and reverse osmosis, the temperature sensitivity would force the reverse osmosis solution distillation would likely require elevated temperatures.

Step (iii): Enter the resulting separation task into the notation for downstream analysis and mapping. $S_{x,NC}$ represents the array containing stream information, where x is the stream count. An accompanying mapping vector, s is also populated during this step.

For a separation task w, performed on $S_{x,}$, place the overhead products in the S_{x+1} vector and bottoms products in the S_{x+2} vector.

Step (iv): Assign an order of separation to the streams. Initial order is unity and $s_1 = 0$. Top and bottom streams increment order positively and negatively respectfully. O is an arbitrary increment for order, and can be set to unity.

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$$if\ s_y = 0:\ s_x = s_y + O, \qquad s_{x+1} = s_y - O, \qquad O^+ = O^- = O = O/10$$

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$$if\ s_y > 0:\ s_x = s_y + O^+, \qquad s_{x+1} = s_y - O^+, \qquad O^+ = O^+/10$$

$$if\ s_y < 0:\ s_x = s_y + O^-, \qquad s_{x+1} = s_y - O^-, \qquad O^- = O^-/10$$

Remark: If the system is not binary (more than two components), iterate and repeat the process.

$$y = y + 1$$

$$x = x + 2$$

The following relationships between purified components, z stream count, x and separation task count, w can be observed.

$$w = y - z$$

$$2w = x + 1\,, \qquad 2w - 1 = x$$

2.2.2 Process Synthesis

For more complex systems process synthesis of a technically feasible flowsheet may be preferred. The methodology is structured so that the algorithm is indifferent to the process synthesis technique applied, if the relevant information is generated. Again, the resultant pathway is the translated into a pre-defined data structure. Technical feasibility is assessed in the following step.

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Algorithm 2.2: Process synthesis

Objective: Obtain physically feasible flowsheet

Step (i): Assign numerical values to the components and parameters. Write the input parameter matrix $I_{i,j}$ (of dimensions $i = NC \cdot NP, j = 2$) for all required components and parameters in the following format, with parameters p, and components c, column one and two ($j = 1, j = 2$) respectively.

$$I_{i,1} = I_{i-NC,1} + 1 \qquad for\ i = NC + 1, NC + 2, \dots, NC \cdot NP$$

$$I_{1,1}, I_{2,1}, \dots, I_{NC,1} = 1$$

$$I_{i,2} = I_{i-NC,2} \qquad for\ i = NC + 1, NC + 2, \dots, NC \cdot NP$$

$$I_{1,2}, I_{2,2}, \dots, I_{NC,2} = 1,2, \dots, NC$$

Step (ii): Populate the input matrix's third column ($j = 3$) with the property values associated with the parameter and component from the preceding two columns. If information not available in literature, generate properties in using a group contribution estimation method. Apply operating conditions to property correlations (such as vapor pressure) to satisfy the remaining required information for $I_{i,j}$.

Step (ii): Perform preferred process synthesis technique. In this case, the method based on thermodynamic insights is preferred for its simplicity. Refer to detailed framework instructions here (Jaksland *et al.*, 1995).

Step (iii): Output the results in the standard notation outlined in Algorithm 2.1 Step (iii & iv).

2.3 Layer 3: Feasibility assessment

In this section of the framework the objective is to quality check the decisions made by the separation selection methodologies. The technical feasibility of the resultant flowsheet of the process synthesis algorithm is first verified. This step is integrated into the technology database generation algorithm, and thus can be bypassed by that framework branch. Both branches then converge before being subjected to a surface level financial assessment tasked in further narrowing the field of candidate cases.

2.3.1 Process verification

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Unfortunately, unlike physical feasibility it is impossible to automatically assess technical feasibility. Due to dependencies on other properties or physical features, some separation tasks generated by the process synthesis framework branch may be unsuitable or impractical. Therefore, should be subject to a manual inspection. Here the user should apply their own knowledge with that of literature, to verify the suggested separation tasks can be suitably achieved using an established technology and at reasonable operating conditions.

Algorithm 3.1: Process Verification

Objective: Plot the ordered pathways, and screen inappropriate tasks

Step (i): Check that each profitable separation task is technically feasible via a literature search. Determine separation barriers such as the presence of mutual solubility or binary azeotropes. If infeasible, exit algorithm to decision gate C, revert back to the separation technology selection of the relevant task. Progress to step (ii) once all identified tasks in the separation pathway have been assessed as suitably feasible.

Step (ii): Assess the technology readiness level of each separation technology comprising the feasible flowsheet. If technology readiness level is below user threshold, exit algorithm to decision gate C, revert back to the separation technology selection of the relevant task. If Technology Readiness Level (TRL) is sufficient for all technologies proceed to step (ii).

Step (iii): Plot the streams and associate separation tasks as per the standard notation outlined in Algorithm 2.1 Step (iii & iv).

Decision Gate C

If the task has an unsuitable TRL or is deemed technically insufficient, revert to back to the separation technology selection and eliminate the task from contention. Proceed with the next most physically feasible task in the separation pathway. If all separation tasks are deemed technically feasible proceed to algorithm 3.2, economic assessment.

Economic Assessment

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Now that the separation pathway is comprised of physically and technically feasible separation tasks, the flowsheet should be assessed for its economic viability. As the most thermodynamically feasible separation tasks require the smallest driving force, it can be assumed that the flowsheet has the lowest OPEX on a relative basis. However it is important to note that this may not be the case, especially if the OPEX of a certain separation technology is significantly cheaper (for a given driving force). The economic assessment algorithm therefore assesses the CAPEX comparison (on a relative basis) of the separation pathway candidates. The Taylor method (Taylor, 1999) is suggested as it facilitates a rapid comparison without requiring significant information input, but other cost estimation methodologies may be applied. A method to evaluate the cost of maturing technologies to an appropriate technology readiness level has been developed and is presented in the supplementary material.

Algorithm 3.2: Economic Assessment

Objective: Screen clearly financially insufficient separation tasks

Step (i): Calculate potential value, V_x of each stream by performing a mass balance on the respective constituents, and applying the component price, pp_i. The case of 100% separation purity assumption is shown as follows. m_x is the mass flow of stream x, F is plant flow capacity, and $\sum_i S_x(C_i)$ is the overall mass fraction of the flow through the separation task.

$$m_x = F \cdot \sum_i S_x(C_i) \ , \qquad V_x = m_x \cdot \sum_i pp_i \ , \qquad for\ x = 1,2,\dots,(2NC-1)$$

Step (iii): Determine the task's throughput, Th_w to calculate the minimum capital cost, Ca_w via the Taylor method [16]. Apply minimum coefficients. Calculate the potential value of the components exiting the separation task.

$$Th_w = m_{2w-1} + m_{2w} \ , \qquad for\ w = 1,2,\dots,(NC-1)$$

$$Ca_w = k \cdot 1.3^{CS_w}(Th_w)^{0.39} \ , \qquad for\ w = 1,2,\dots,(NC-1)$$

$$Va_w = V_{2w-1} + V_{2w} \ , \qquad for\ w = 1,2,\dots,(NC-1)$$

*If a separation task in the case is not TRL 9, determine the required development cost for full

implementation. Perform $for\ w = 1,2, \dots, n$.

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$$DEV_w = 10 \cdot k \cdot 1.3^{cs_w} (Th_w)^{0.39} (0.965 - 0.0171 \cdot TRL_w^2 + 0.0433 \cdot TRL_w)$$

Step (iv): Determine the payback period of the task.

$$Pb_w = \frac{Ca_w + Dev_w}{Va_w}$$

Decision Gate D

If the payback period generated from the combined value of the streams existing the studied separation task and the capital cost, is greater than the threshold set by the user, the pathway is omitted. Revert to the separation selection section and assign the next most promising component as the target for recovery.

2.4 Layer 4: Techno-Economic Evaluation

If the user intends only on an order of magnitude estimate of the Net Present Value, process approximation methods should also be applied to determine the associated operating costs. For more detailed assessments, process simulation is suggested. Once simulated, the model can be applied to determine recoveries, equipment costs, and operational expenses, ultimately resulting in improved NPV accuracy. If financially satisfactory, the framework is concluded with application of the WAR algorithm [17] application to ensure environmental compliance. At this point the user should have a clear picture as to whether or not to pursue investment.

Option Gate E

If an order of magnitude estimate is desired, apply algorithm 4.3. Apply algorithm 4.1 & 4.2 for a more detailed assessment.

2.4.1 Process Simulation

The intention of the process simulation framework step is to highlight any overlooked infeasibilities and provide the required information for the subsequent economic analysis. The simulation can be viewed as a comprehensive mass and energy balance, generating the product flows, process unit throughputs, utility duties, and process inflows as an output. Therefore, the process simulation software applied is inconsequential.

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Algorithm 4.1: Process simulation

Objective: Obtain mass and energy balances

Step (i): Simulate the successful case flowsheets in the user's process simulation software of choice. Use the inbuilt palette units to model the separation tasks. Adjust process conditions iteratively using utility units (heaters, coolers, pumps, etc.) to those required for complete separation.

Note: If the separation task cannot be simulated via an inbuilt palette unit, mimic experimental results found in literature with a component splitter. Emulate the experimental process conditions with utility units. Determine splits with retention, R and separation factors, X. Where, c_p and c_f are product and feed concentrations respectively.

$$R_A = 1 - \frac{c_{p_A}}{c_{f_A}}, \qquad R_B = 1 - \frac{c_{p_B}}{c_{f_B}}, \qquad X_A = \frac{(c_{p_A}/c_{p_B})}{(c_{f_A}/c_{f_B})}, \qquad X_A = \frac{1 - R_A}{1 - R_B}$$

Note: If a transport medium or mass separating agent is required, introduce the stream to the process via mixing units. Adjust the operating conditions to those required to exploit the benefit of the mass-separating agent (e.g. set temperature to azeotropic boiling point).

Note: Introduce recycle units and recirculate waste streams if applicable. Avoid unsatisfactory accumulation by setting makeup and purge streams flowrates and concentrations accordingly. Adjust conditions until the recycle loop converges suitably.

Note: If a reaction occurs and the condition dependent rate kinetics are known, simulate with the inbuilt palette reactor units. If the reaction is complex or is biological, model with a conversion reactor using experimental results found in literature.

Step (ii): Once the process is simulated, record the target component outlet flows (and concentration), supplementary inlet flows, unit relative throughputs, and utility duties for application in algorithm 4.2.

Economic analysis

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At the point in the framework, preliminary economic screening has been applied but any significant analysis is yet to have occurred. Net present value, or NPV is chosen as the evaluation method as internal rate of return does not work well with long project periods or uncertainties (Peters *et al.*, 2003). NPV gives the present value of all payments and provides a basis of comparison for projects with different payment schedules but similar lifetimes. Using the outputs of the process simulation section the OPEX and CAPEX can easily be estimated using the suggested methods (utility summation and Taylor CAPEX method (Taylor, 1977)), else the users preferred technique should be applied.

<u>Algorithm 4.2: Economic analysis</u>

Objective: Identify most profitable case

Step (i): Specify discount rate, technology readiness level, investment period, and minimum return threshold. This evaluation will be carried out as per the description of [12]

Step (ii): For each case, calculate annual revenue and operating expenditure with the results of algorithm 4.1, and discount the difference to a present value. c refers to the case being evaluated, t refers to a specific target component.

$$OPEX_c = W_c + D_c + C_c\,, \qquad Rev_c = \sum T_{c,t} \cdot F_{c,t}\,, \qquad for\ c = 1,2,\dots,n$$

$$PV_c = (Rev_c - OPEX_c) \cdot \left(\frac{1-(1+dr)^{ip}}{dr}\right), \qquad for\ c = 1,2,\dots,n$$

Step (iii): If a proper equipment sizing and equipment cost estimation procedure is an option, apply it. Otherwise, apply the relative throughputs determined in algorithm 4.1 to the Taylor methodology of calculating capital cost of the cases. w refers to the separation task being assessed.

$$CAPEX_c = k \cdot \sum 1.3^{cs_{c,w}} \left(Th_{c,w}\right)^{0.39}\,, \qquad for\ c = 1,2,\dots,n$$

Note: If a separation task in the case is not TRL 9, determine the required development cost for

full implementation. Perform $for\ c = 1,2,\dots,n$.

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$$DEV_c = 10 \cdot k \cdot 1.3^{cs_{c,w}} \left(Th_{c,w}\right)^{0.39} \left(0.9465 - 0.0171 \cdot TRL_{c,w}^2 - 0.0433 \cdot TRL_{c,w}\right)$$

Step (iv): Compute the net present value for each case.

$$NPV_c = PV_c - CAPEX_c - DEV_c\,, \qquad for\ c = 1,2,\dots,n$$

Step (v): Supplement NPV as a financial decision metric by subjecting the cases to further payback period and return on investment analysis.

$$PB_c = \frac{CAPEX_c + DEV_c}{PV_c/pp}\,, \qquad ROI_c = \frac{NPV_c}{CAPEX_c + DEV_c}\,, \qquad for\ c = 1,2,\dots,n$$

2.4.2 Process Approximation

In the interest of efficiency, the user may decide not to pursue a complex process simulation and instead desire an order of magnitude estimate of the profitability. Regardless of the path taken by the framework, a simplistic estimation of the capital cost is generated in algorithm 3.2. In order to supply algorithm 5.1 with the required information the associated operating costs must also be approximated. This can be done via the suggested method or by the users preferred technique.

Algorithm 4.3: Process approximation

Objective: To find the order of magnitude of the resource recovery net present value

Step (i): CAPEX is known from algorithm 3.2, apply OPEX estimation method or the users preferred technique.

Step (ii): Continue from algorithm 4.2 step (iv).

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Decision Gate F

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If both financial metrics are above the set threshold, investigate further via the pursue investment framework step. If more than one case is greater than the thresholds, Th^{npv} and Th^{pb}, select the case with the highest NPV.

$$if\ PB_c < Th^{pb}\ \&\ ROI_c > Th^{roi}\ \&\ NPV_c > Th^{npv}:$$

$$Th^{npv} = NPV_c, \qquad investigate\ c\ , \qquad for\ c = 1,2,\dots,n$$

If no cases meet the threshold requirements, the pathway is omitted. Revert to the separation selection section and assign the next most promising component as the target for recovery. If all components have been assessed, exit the framework.

2.4.3 Pursue Investment

Due to the nature of the framework requiring multiple approximation techniques it should be noted that the outcome of algorithm 4.2 be viewed as a relative recommendation amongst the candidates and further work must be done to verify profitability and environmental compliance. The first step of this confirmation process is undertaken in algorithm, where key metrics are subject to sensitivity analysis, and the environmental impact further evaluated with the WAR algorithm (Young and Cabezas, 1999). Future planned developments of this project include a comprehensive integration of uncertainty analysis along the framework.

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<u>Algorithm 5.1: Pursue investment</u>

Objective: Confirm investment decision by investigating environmental effects and performing sensitivity analysis

Step (i): Isolate the points along the framework that contribute the highest degree of uncertainty and subject them to sensitivity analysis. This can be done by varying these key metrics above and below their applied value and observing the effect upon the decision metrics; ROI and Payback.

Step (ii): Perform the WAR algorithm (Young and Cabezas, 1999) or any other suitable

methodology to assess the environmental impacts on the successful candidate to evaluate its sustainability.

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Decision Gate I

If investment confidence is reassured by applications of sensitivity analysis and the WAR algorithm (Young and Cabezas, 1999), move to next steps of project development. If the outcome of the pursue investment framework step does not inspire confidence, investigate the offending aspects accordingly.

Important to notice is that that the use of the WAR algorithm has been mainly proposed for simplicity, since it is mostly an outdated process. The authors suggest to consider the use of this method in a relative or comparative perspective to narrow down the search space.

3. Software Implementation

3.1 Motivation

Upon reflecting on the finished framework, it was clear that the efforts to uphold comprehensiveness could potential be perceived as a downfall, in respect to the number of challenges that arise when attempting to apply manually, namely the complexity and time it takes to apply. This is an unintended consequence, as the framework was envisioned to aid users quickly through the resource recovery potential identification process. Consequently, computer aided functionalities were deemed as a necessary addition to streamline the process, thus TaskGen was conceived.

3.2 Overview

TaskGen is a tool created to aid users through the conceived resource recovery framework. When using the tool many of the aforementioned framework steps can be completed rapidly with use of the tool, thus drastically decreasing complexity and increasing ease of application. TaskGen facilitates swift generation of feasible flowsheets, thus allowing users to assess possibilities that may not have been previously considered, and eliminate unsuitable candidates early the evaluation process. An illustration of how framework implementation is assisted with the use of TaskGen can be seen in Figure 3.

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3.3 Implementation

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A condensed framework has been generated to be used in coordination with TaskGen. No new concepts or operations are presented, instead, a result orientated framework guidance methodology is proposed, facilitating use of the framework at an increased rate and accuracy. To achieve this, the functionalities of TaskGen are specifically designed to perform the most arduous and complex algorithms in the framework, such as the separation selection step. For sake of brevity the condensed framework, installation & case set-up guide, source code, and in-depth examples are available upon request.

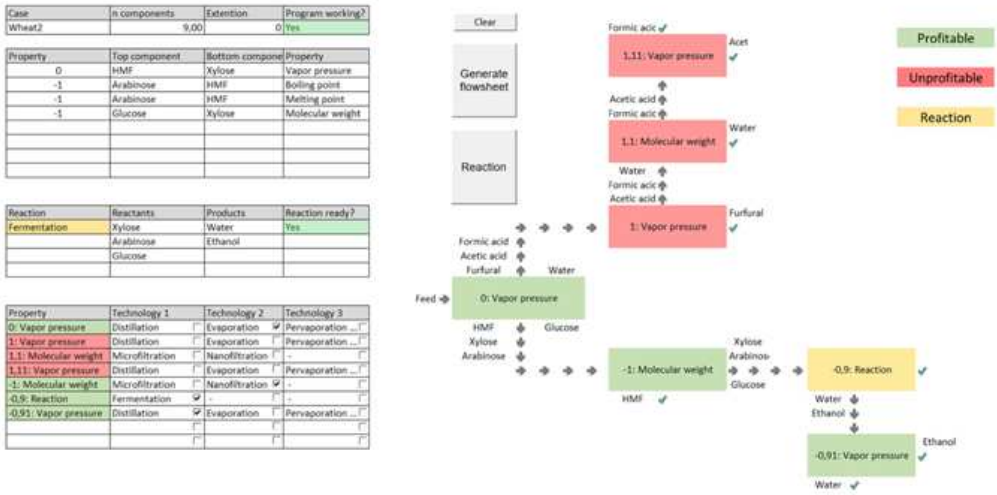

Figure 3. TaskGen central dashboard. Ethanol production case presented

4. Case Study: Wheatstraw Biorefinery

Now that the separation selection methodology has been established, a demonstration example of framework implementation can be presented. A wheat bio refinery process was selected due to the fact that its 'waste' stream provides opportunity to demonstrate the full functionality of the framework. A small to medium sized wheat bio refinery has been hypothesized, with a flow capacity of 30 kilotons per year of concentrated pre-treatment liquor.

4.1 Potential Identification

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4.1.1 Problem Formulation

The solution strategy was viewed from a decomposition perspective, and focus was set on the financial, technological, and environmental aspects. Throughout the framework algorithms, financial constraints are applied to the potential candidates, manifested as payback and return on investment thresholds. Technological constraints are implemented in the form of technology readiness level. The environmental constraints are expressed as maximum environmental impact category thresholds of the Danish standards (Ministry of environment and food of Denmark). If more than one candidate successfully suffices these constraints, the decision to pursue further investment investigation relies upon the maximum NPV and ROI.

$$\max f(NPV, ROI)$$

$$subject\ to:$$

$$GSP \geq \frac{20\$}{m^3}, \qquad Payback\ \leq 5years\,, \qquad TRL \geq 7, \qquad ROI \geq 50\%\,,$$

$$Environmental\ impact\ \leq Danish\ standards$$

4.1.2 Waste Characterization

Table 1. Pre-treated wheat straw stream components. Capacity, 30 [kt/yr]

I	Compound	Formula	MW	Concentration
a.	Acetic acid	CH_3COOH	60	12.34
b.	Formic acid	CH_2O_2	46	2.14
c.	Furfural	$C_5H_4O_2$	96	4.22
d.	HMF	$C_6H_6O_3$	126	0.63
e.	Xylose	$C_5H_{10}O_5$	150	58.20
f.	Arabinose	$C_5H_{10}O_5$	150	8.46
h.	Glucose	$C_6H_{12}O_6$	180	14.03
i.	Water	H_2O	18	900

Table 2. Generated cases for wheat biorefinery process stream

Recovery Product	Reaction	Constraints	Case
Initial components	None	None	1
Ethanol	Yes (Fermentation)	Inhibitors	2

The algorithm provides two cases worthy of further investigation.; extraction of the initial components and the production and separation of ethanol.

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The studied process stream results from the hydrothermal pre-treatment of wheat straw (Oskay, 2007). The liquor form the pre-treatment was then concentrated, resulting in a dissolved solid concentration of 100g/L. The hydrothermal processing occurred in the pilot-plant reactor "Mini IBUS" at the Technical University of Denmark (Ambye-Jensen *et al*., 2013). High performance liquid chromatography was performed to determine the concentrations of the pre-treatment liquid stream, shown in Table 1**Error! Reference source not found.**.

The target stream characterization algorithm was performed to generate a list of recovery scenarios. A literature search was undertaken to evaluate if each compound is commonly reacted or acts as an inhibitor. It was determined that moderate concentrations of acetic acid, formic acid, furfural, and HMF inhibit the widely practiced conversion process of monosaccharide's to ethanol via fermentation (Sueb, 2017). Therefore, there are two cases to be examined; initial component recovery and fermentation product recovery, as seen in *Table 2*. The first case shall be covered comprehensively in this section whilst the second case can be supplied by request.

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4.1.3 Gross sustainability potential

Target compounds xylose and arabinose were identified as a result of performing the economic potential algorithm, shown in *Table 3*. Yearly economic potential from recovery of these two monosaccharides is estimated to be $13.4MM.

Table 3. Economic potential preliminary value breakdown (concentration normalized). Produced from algorithm 1.3

Component	Price $/m^3	CO2 cost $/m^3	Treatment cost $/m^3	GSP $/m^3
Acetic acid	5.55	0.72	4.74	11.01
Formic acid	1.07	0.08	0.27	1.42
Furfural	5.06	0.39	2.53	7.98

HMF	6.27	0.05	0.34	6.66
Xylose	215.34	3.41	22.35	241.10
Arabinose	232.55	0.50	3.25	236.29
Glucose	7.01	0.82	5.39	13.22
Water	2.49	0.00	0.00	2.49

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As they exceed the user set threshold value of \$20.0/m^3 progression through the framework is continued.

The unit prices for the components in the wheat straw pre-treatment liquid were identified via online marketplaces. A similar bioethanol effluent stream originating from wheat straw uses an up flow anaerobic sludge blanket reactor for detoxification of the process water [18]. The treatment unit cost associated with up flow anaerobic sludge blanket reactor operations is found to be $\$0.36/kgCOD_{removed}$ at 80% removal [19]. The economic sustainability influencing factors are converted to \$/m^3 units and combined to form a total value in *Table 3*.

Decision gate A

The results of performing the economic potential framework step are illustrated in *Table 3* present clear target components, arabinose at \$236.3/m^3 and xylose at \$241.1/m^3. The rest of the process stream constituents do not meet the \$20.0/m^3 threshold value set, thus are deemed economically insufficient and are not targeted for removal.

4.2 Separation Technology Selection

Option Gate B

Process synthesis techniques are applicable in this case, thus algorithm 2.2 is proceeded with (algorithm 2.1 bypassed). The Jaksland method based on exploiting thermodynamic insights was chosen in this instance (Jaksland *et al*., 1995). Implementation of Jaksland was undertaken with TaskGen assistance (see software implementation section).

4.3 Process Verification

4.3.1 Process Synthesis and Process Verification

Process synthesis and process verification (algorithms 2.2 and 3.1) occur simultaneously within TaskGen, thus their demonstration shall be illustrated concurrently.

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The final flowsheet obtained by performing both the process synthesis and verification framework algorithms in TaskGen is illustrated in *Figure 4*. The progression of the separation pathway passes is visualized in *Figure 4*.

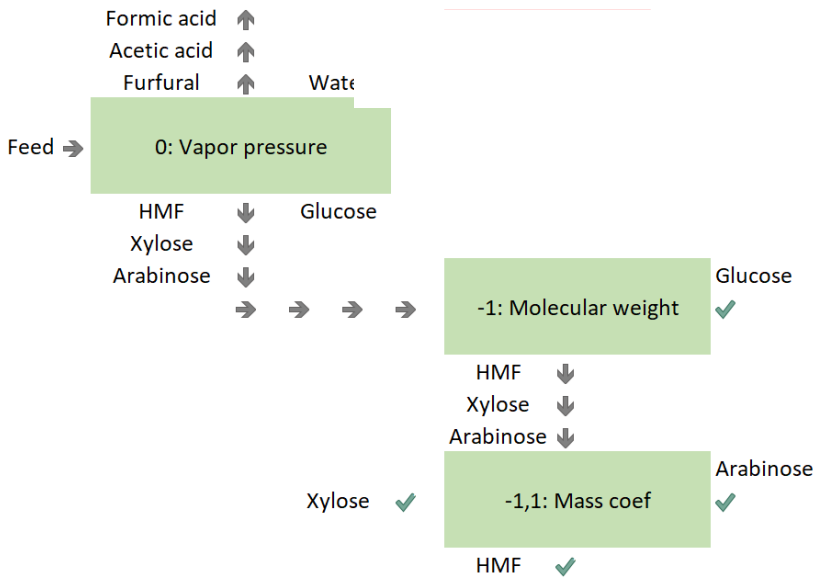

Figure 4. TaskGen facilitated framework fifth (final) pass.

Framework pass 1

Tasks 1.0, 1.1, and 1.11 are unable to produce an acceptable payback period irrespective of the chosen separation technology, due to the economic insight framework step, thus the pathway is neglected (Refer to figure 3 for further clarification) Conversely, tasks 0, -1.0, and -1.1 illustrate promising economics.

- Task 0: It is not possible to distil HMF from the solution, as it is prone to thermal degradation [20]. Using TaskGen, the respective binary pair boiling point and vapour pressure ratios was set to zero and a second pass was run, resulting in a second pass.

Framework pass 2

Despite lowering the process temperature and retaining furfural, the positive pathways are still deemed economically insufficient for all technologies by the economic insights examination. Therefore, the

associated streams are excluded from the remaining analysis. The other tasks continue to have promising economics.

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- Task 0: Furfural separation via evaporation is feasible and often applied in hydrolasate detoxification procedures [21]. Moreover, as furfural forms an azeotrope with water, the water component must partake in the separation technology selection process rather than observe as a transport medium.
- Task -1.0: HMF crystallization is possible but is generally undertaken as a purification step and requires significant solvent addition [20]. Using TaskGen the respective binary pair property ratio was set to zero and a third pass was run, resulting in a third pass.

Framework pass 3

All tasks illustrate promising economics.

- Task -1.0: Glucose separation is possible with the use of a spiral wound nanofiltration membrane [22].
- Task -1.1: HMF separation from monosaccharaides using a liquid membrane is possible, but at a low TRL [23]. Moreover, eutectic solvents are expensive and difficult to regenerate. Using TaskGen the respective binary pair property ratio was set to zero and a fourth pass was run, resulting in a fourth pass.

Framework pass 4

All tasks illustrate promising economics.

Task -1.1: HMF separation from monosaccharide's is possible with nanofiltration [24]. Moreover, for the purposes of monosaccharide concentration, reverse osmosis is advantageous.

- Task -1.09: Arabinose separation from xylose is difficult due to their similar structure. However, it is possible with chromatographic adsorption using a cation exchange resin [25]. Whilst, this separation technique is industrially established, it is not at an industrialized scale for the purposes of monosaccharide extraction, thus was given a TRL equivalent to 7 as the relevant system has not completed and qualified through test and demonstration [26]. This TRL is suitable as per the user set thresholds. During the literature review, it was discovered that low concentrations of HMF have a

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negligible effect on ion exchange separation [25]. Task -1.1, is therefore deemed unnecessary in the flowsheet and removed via setting the respective binary pair property ratio to zero in TaskGen, and running a fifth and final pass in TaskGen, as seen in *Figure 4*.

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Framework pass 5

All negative tasks illustrate promising economics.

- All tasks have now undergone feasibility assessment; thus, the refined flowsheet can be seen in *Figure 4*.

Decision Gate C

All tasks in *Figure 4* were suitably identified as technically feasible via literature search. The tasks TRL's also met user set threshold.

4.3.2 Economic Assessment

The results of performing the economic elimination framework step on each task generated on each TaskGen pass can be seen in *Figure 5*.

Figure 5. Monosaccharide extraction case. Economic sufficiency of each task generated by TaskGen. An empty bubble indicates that this task was not assigned for the associated pass.

It is evident from *Figure 5* that at no point did the separation pathways comprised by the positive (overhead) tasks came close to illustrating sufficient economics and were therefore eliminated. Conversely, every negative task had sufficient economics and passed Decision gate D to the process simulation framework step.

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Decision Gate D

The payback period generated from the combined value of the streams existing the studied separation task and the capital cost, is greater than the user set threshold set by the user, therefore the framework is continued to the techno-economic evaluation step.

Option Gate E

A more detailed assessment for desired for this case, thus the framework pathway of algorithms 4.1 & 4.2 was chosen.

4. 4 Layer 4: Techno-Economic Evaluation

4.4.1 Process Simulation

The process simulation of the monosaccharide extraction and ethanol production cases can be seen in *Figure 6*. *Table 4* and *Table 5* illustrate the target component recovery and required duty's for each case.

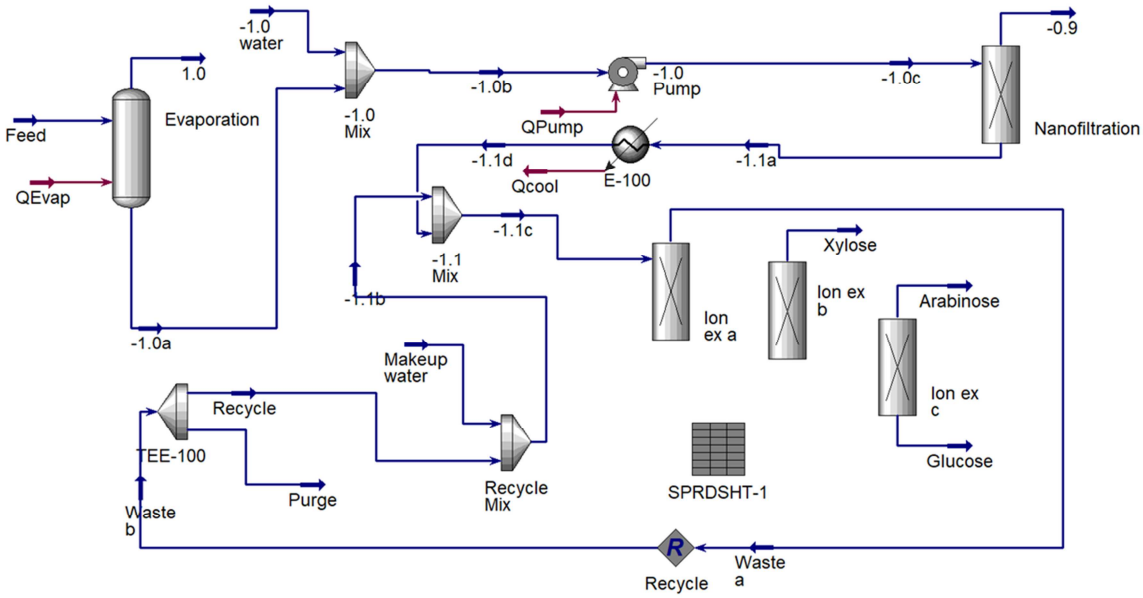

Figure 6. Mass and energy balance for wheat biorefinery monosaccharide extraction case

Table 4. Target component flow and recovery for monosaccharide extraction case

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Case	Target	Flow	Recovery
1	Xylose	16.36 kg/hr	56.5%
1	Arabinose	86.79 kg/hr	43.6%

Table 5. Heating and electrical duty's for monosaccharide extraction case

Case	Heating duty	Electrical duty
1	7.92 GJ/hr	17,4 kw

Aspen HYSYS was chosen as the simulation tool because of its user friendliness, thus enabling quick generation of system balances. Common operations such as evaporation were modeled with the inbuilt palette blocks, whilst tasks such as nanofiltration were emulated with the component splitter. Care was taken to match the conditions and separability of each task simulated with information found in literature. The resulting mass and energy balances shown in *Table 4* and *Table 5* were applied to determine the OPEX in the following economic analysis section.

Economic Analysis

The discount rate and project duration for the studied cases have been set at 10% and 10 years accordingly. The adsorption unit of the monosaccharide extraction has been set to TRL 7, whilst all other operations have assumed TRL 9. The operating cost, capital cost, and net present value analysis can be seen in *Table 6*, *Table 7* &, and *Table 8* respectively. The metrics to be applied to the following decision gate, payback period and return on investment can be seen in *Table 9.*

Table 6. Operating cost and revenue analysis in USD. Flow bases 30 [kt/yr]

TRL	Water cost	Power/heating	Consumables	Revenue	Total
8.33	-13,122	-277,600	-255,800	6,916,621	6,370,099

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Table 7. Monosaccharide extraction capital cost estimate (Taylor method) in USD [16]. Flow bases 30 [kt/yr]

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Task	Throughput	Throughput score	Technology score	Total score	Capital cost
0: Evaporation	12,39	4,7	2	6,7	-3,976,000
-1.0 Membrane	3,05	2	4,8	6,8	-2,363,000
-1.1 Adsorption	2,65	1,7	4,4	6,1	-1,862,000
Cumulative					-8,202,000

Table 8. Net present value analysis in USD. Flow bases 30 [kt/yr]

Present value	Capital cost	Development cost	Net Present value
39,141,000	-8,202,000	-11,0210,00	19,618,000

Table 9. Return on investment and payback period values

Return on investment	Payback period
1.02	4.99

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As it can be seen in *Table 8* and *Table 9*, monosaccharide extraction provides positive economic return. The mass and energy balances performed in the process simulation section were applied to determine utility duties, which were combined and discounted to produce the OPEX. This was then combined with the discounted revenue to produce the present value of the project. Capital costs were again estimated for each process technology by applying the Taylor method (Taylor, 1977), as seen in *Table 7*. Rather than applying the minimum complexity scores, as done in the economic assessment section, individual scores are computed and applied to provide an accurate estimation. Development cost of the adsorption unit was determined using the developed technology readiness level correlation. Once all monetary facets combined, the resultant net present value is realistic and illustrates promise.

Decision gate F

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Both required financial metrics meet the user set thresholds, and the framework continues to the pursue investment section. The thresholds were a 50% return on investment and 5 years payback period respectively.

4.4.2 Pursue Investment

Several key framework nodes were identified to possess high uncertainty; market price, adsorption unit TRL, and capital cost estimation. To this end, the influence of these factors must be considered in detail to arrive at a practical conclusion. It was decided to perform sensitivity analysis on these three factors separately and their results displayed in Figure 8, *Since the* price of monosaccharide was taken from an online commodity marketplace, the sensitivity of the net present values to the unit price of the products can be analyzed where is shows the overall Net Present value of the project can breakeven with a 45% drop in the market price. While this manuscript did not look at the market volatility of monosaccharide, it can be reasonably assumed that a 45% reduction in a commodity product over a short to a medium period is unlikely.

Table 10, and **Error! Reference source not found.**. In addition, environmental considerations of the developed processes were evaluated in detail via application of the WAR algorithm, as illustrated in Figure 9.

Figure 7. Price sensitivity analysis

Since the price of monosaccharide was taken from an online commodity marketplace, the sensitivity of the net present values to the unit price of the products can be analyzed where is shows the overall Net Present value of the project can breakeven with a 45% drop in the market price. While this manuscript did not look at the market volatility of monosaccharide, it can be reasonably assumed that a 45% reduction in a commodity product over a short to a medium period is unlikely.

Table 10. Effect of monosaccharide adsorption TRL on NPV in USD

Adsorption TRL	Development Cost	Net Present Value
7	-11,0210,00	19,618,000
6	-17,774,000	13,165,000
5	-23,914,000	7,025,000

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Table 10 illustrated the economic effect of incorrectly estimating the TRL of the adsorption unit operation which is a key part of the monosaccharide, where it can be seen that the overall project NPV can be reduced by over 60% simply due to changing the TRL allocation for the Adsorption unit from the TRL of 5 (Mid Pilot) to a TRL value of 7 (early full scale). While in this case this differing TRL did not result in a negative NPV, it can be seen that incorrectly assigning a TRL (+/- 2 levels) even for a single unit operation can result in a reversal of NPV based economic feasibility.

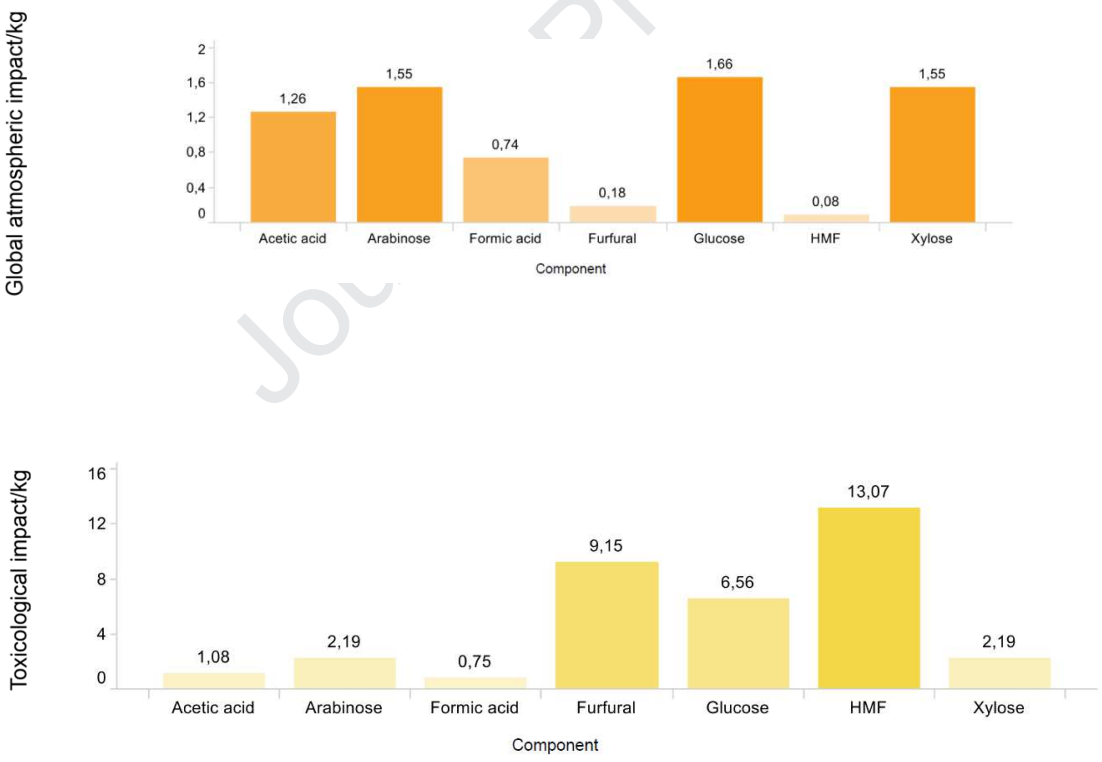

Figure 9. Global atmospheric and local toxicological potential environmental impact. Produced from the

To understand the overall environmental impact of the proposed production process, the WAR algorithm (Young and Cabezas, 1999) was employed, the results obtained can be seen in Figure 9 where it can be seen

that from a toxicological perspective some hazardous components are present in low concentrations, specifically HMF and furfural. However, when the impacts of these compounds normalized to their respective process stream concentration, the overall impact of these compounds are insignificant in comparison to the compounds present in high concentrations. Moreover, the global atmospheric impact values for all compounds are significantly below levels of concern. Therefore, it can be said that no apparent environmental impact would block a potential investor to proceed to further detailed engineering design and investigation for the proposed project.

Implications

The application of the developed computer-aided methodology to the case study illustrates the apparent benefits of systematically tackling a multi-faceted, multi-disciplinary and multi-scale set of challenges that must be overcome when developing industrially applicable resource recovery projects. It is also clear that the decisions made in the first parts of the framework have a knock on impact on the process design. To this end not considering the global level issues which goes beyond the plant/process bounds, hence typically not a part of the engineering design processes must be implicitly considered in the resource recovery project development process. Based on the case study, it can also be seen the strong influence TRL has on the economic viability of a given project, to this end there is a clear and apparent need to implicitly consider TRL when developing resource recovery projects as not considering these aspects clearly leads to solutions that on paper has a high NPV but when considering the significant development costs that are required means they are infeasible. To this end, the framework proposed suggest a practical framework that can be followed.

It is also important to note that for projects where the TRL of a novel unit operation jeopardizes its positive economic outcome and there are no other higher TRL options available, the apparently cost of development can be reduced by spreading out the development cost over a several projects. This particularly becomes a practical and viable option if similar waste streams are found in more than one location, which means once the technical development is done ten similar projects can be implemented. However, this raises another issue which is the requirement to secure the sufficient funds to carry out the technical development work necessary which can be a complex and challenging endeavour.

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On a positive note the case study as well as the framework developed allows investors to focus on resource recovery projects that are likely to have a positive NPV outlook, which increases the chances of project implementation and allows the domain of resource recovery as a whole to move towards implementation space.

5. Conclusions

In this work, a systematic computer-aided framework has been developed to evaluate the techno-economic aspects and the environmental potential of resource recovery initiatives. The framework application has been demonstrated on a wheat bio-refinery case study where it was employed to identify and develop solutions in the presences of multiple target resources, and facilitate generation of lucrative technically feasible separation pathways. It is important to underline that this framework is not a decision-making tool. The framework itself is a support system that offers a solution strategy to overcome the barrier of multidimensional problems, thus assisting providing solutions and justifying choices. In future, more research needs to be carried out on application of the concepts outlined in this framework while making necessary changes and adjustments to the other methodologies used in this context. Furthermore, complete utilization of such approach also depends on better information flow between different stakeholders at industrial, societal and policy making sectors which are enabled by this framework.

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Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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