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*Research Article*

# Green Chemistry in the Hydrolysis Process of Cellulose by Acids: Modelling, Optimization, and Life Cycle Assessment

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**Abstract**

Cellulose is a critical material in a variety of engineering applications, holding significant importance in the evolving landscape of future lifestyles. The imperative for its production in the future is underscored by its versatile utility. However, conventional production processes involve the application of numerous chemicals. In this research, MATLAB-based simulation played a pivotal role in modeling the hydrolysis process during cellulose production. We further extended the simulation to optimize the production process. Notably, the application of life cycle assessment (LCA) brought an additional layer of sustainability to the study, resulting in the development of a more environmentally sound and sustainable acidification method for the hydrolysis process. This integrated approach holds promise for fostering a more sustainable and eco-friendly future in cellulose production.

**Keywords**: Cellulose; Green Chemistry; Hydrolysis Process; Optimization; Life Cycle Assessment

## INTRODUCTION

Green chemistry has emerged as a pivotal approach in the field of chemical processes, advocating for sustainable and environmentally friendly methods. One such application is found in the hydrolysis of cellulose by acids. Cellulose, a complex polysaccharide abundant in plant cell walls, serves as a renewable resource for the production of various valuable products, including biofuels and chemicals. Conventional hydrolysis methods often involve harsh conditions and toxic reagents, leading to environmental concerns and safety issues. The integration of green chemistry principles into the hydrolysis process aims to address these challenges, promoting efficiency while minimizing environmental impact [1]. The hydrolysis of cellulose involves breaking down the complex cellulose structure into simpler sugars through the use of acids. Traditional methods typically employ strong mineral acids, such as sulfuric acid, which not only pose risks to human health but also contribute to pollution. Green chemistry principles emphasize the development of alternative, more sustainable routes. Researchers are exploring milder acid catalysts and environmentally benign solvents to achieve cellulose hydrolysis, aiming for a cleaner and safer process [2].

An essential aspect of green chemistry in cellulose hydrolysis is the focus on reducing waste and energy consumption [3]. Conventional methods often generate large amounts of by-products and require significant energy input. Green approaches aim to minimize waste generation, optimize reaction conditions, and utilize renewable energy sources, contributing to a more sustainable and economically viable process. Furthermore, the implementation of green chemistry in cellulose hydrolysis aligns with the broader goals of the bio-based economy [4]. As society seeks alternatives to petrochemical-based products, cellulose-derived sugars have become crucial feedstocks for sustainable production. Green chemistry ensures that the hydrolysis process aligns with the principles of green and circular economies, promoting resource efficiency and reducing dependence on finite resources [5]. The dynamics of global chemical fiber production from 2000 to 2022, categorized by fiber type and quantified in 1,000 metric tons, are visually depicted in Figure 1. This comprehensive representation offers valuable insights into the evolving landscape of fiber production over the years. Beyond the numerical data, it serves as a pivotal reference point for understanding the shifting preferences and trends within the industry [6]. Within this context, it becomes evident that the production and utilization of chemical fibers are integral components of the larger discourse on sustainable practices. The utilization of green materials in manufacturing processes, as highlighted in the presented scheme, underscores the industry's commitment to environmentally responsible and sustainable approaches. This emphasis on green materials is a critical aspect of the broader global movement toward more eco-friendly and socially responsible industrial practices [7]. The significance of incorporating green materials in chemical fiber production lies in their renewable and environmentally friendly attributes. Embracing materials derived from sustainable sources, such as cellulose from plants, not only addresses concerns related to resource depletion but also mitigates the environmental impact associated with traditional, non-renewable resources. This shift towards green material applications aligns with the increasing awareness of the ecological footprint of industrial processes and the imperative to adopt more sustainable alternatives [8]. Moreover, the depicted trends in global chemical fiber production signify a paradigm shift towards a more conscious and responsible production framework. This transformation is not only reflected in the sheer volume of fiber production but also in the quality of the materials utilized. Green chemistry principles, emphasizing reduced environmental impact and enhanced efficiency, are becoming increasingly integrated into industrial practices, contributing to a more sustainable and circular economy [9].

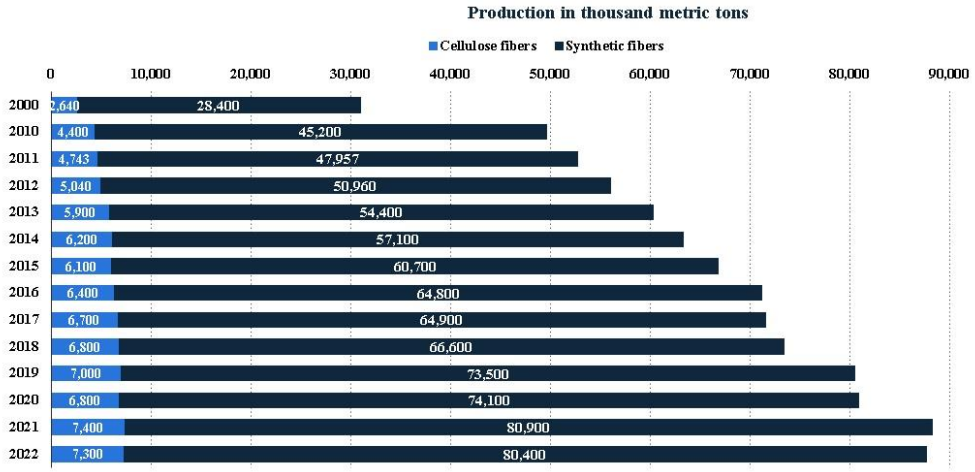


**Fig. 1.** Global production of chemical fibers, categorized by fiber type, spanning from 2000 to 2022 and measured in 1,000 metric tons.

## Methodology

The trajectory of our investigation is meticulously outlined in Fig. 2, elucidating the comprehensive research roadmap for the current study. This visual representation serves as a guide, delineating the sequential progression of key milestones, methodological approaches, and crucial junctures that shape the course of our scholarly exploration. The figure encapsulates the strategic design of our research, offering a visual narrative that not only underscores the interconnectedness of various components but also provides a roadmap for understanding the overarching framework guiding our inquiries.

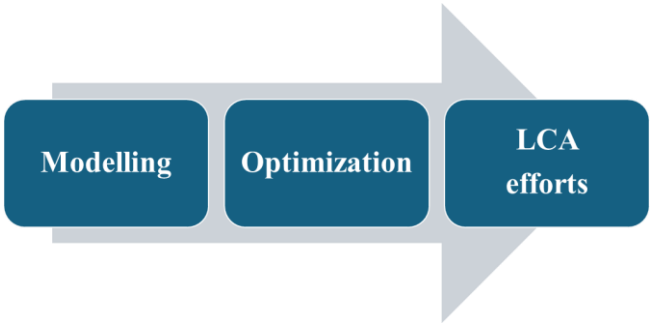


**Fig. 2.** The research roadmap of this study.

### *Modelling of Hydrolysis Process*

In this methodology, the amount of acid needed for the hydrolysis of cellulose in sugarcane bagasse is calculated based on acid concentrations and pH values. The following mathematical equations represent the key calculations involved in the program [10].

Conversion of input parameters to SI units:

*Bagasse_weight = bagasse_weight/1000 (convert bagasse weight to kg)* (1)

*Acid_volume = acid_volume/1000 (convert acid volume to L)* (2)

Calculation of the number of moles of acid used:

*Acid_concentration=acid_concentrations_(i)* (3)

acid_moles = acid_concentration×acid_volume (moles of acid used) (4)

Calculation of the mass of cellulose in the bagasse:

*Cellulose_mass = bagasse_weight×cellulose_density* (5)

Calculation of the number of moles of cellulose in the bagasse:

*Cellulose_moles = cellulose_mass/(molar_mass_cellulose)* (6)

Calculation of the amount of acid needed to hydrolyze the cellulose:

*Acid_moles_needed=2×cellulose_moles (2 moles of acid needed to hydrolyze 1 mole of cellulose)* (7)

Calculation of the excess acid:

*Acid_moles_excess=acid_moles−acid_moles_needed* (8)

Calculation of the pH of the acid solution:

$pH = -\log_{10}(acid\_concentration)$ (9)

These calculations are performed in a nested loop for varying acid concentrations and pH values. The resulting matrix stores the amount of acid needed for hydrolysis under different conditions. The contour plot is then generated based on this matrix to visualize the relationship between acid concentration, pH, and the amount of acid needed for cellulose hydrolysis. The applied program of this section is demonstrated in **Code S.1**.

## *Optimization*

In the methodology section of the code, an optimization approach is introduced to enhance the efficiency of the acid amount calculation for cellulose hydrolysis in sugarcane bagasse. The optimization is performed using the fmincon function, with the objective of minimizing the amount of acid needed. The mathematical equations and steps for the optimization method are detailed below [11].

An objective function, objective_function(x), is defined to represent the amount of acid needed for cellulose hydrolysis. This function takes as input a vector x containing the acid concentration and pH values. The function is defined as:

*Objective_function(x)=acidOptimizationObjective(x,bagasse_weight,acid_volume,cellulose_density,molar_mass_cellulose)* (10)

The fmincon function is employed for the optimization process. The initial guess for the acid concentration and pH is provided as [0.5,2.0]. The optimization is constrained to ensure that the acid concentration remains between 0 and 1, and the pH remains between

0 and 4. The optimized parameters, optimized_paramsoptimized_params, are obtained by minimizing the objective function. The optimized parameters are used to update the acid concentration (acid_concentration_optimized) and pH (pH_optimized) values. The function calculateAcidNeeded is employed to determine the amount of acid needed with the optimized acid concentration and pH values. This result is stored in acid_moles_needed_optimized. The matrix acid_needed_optimized is filled with the optimized acid moles needed, and it is used to create a contour plot representing the optimized conditions. The practical implementation of this section is illustrated in **Code S.2**.

## *LCA analysis*

The Life Cycle Assessment (LCA) method is employed to evaluate the environmental impact of the acid hydrolysis process in the context of sugarcane bagasse conversion to cellulose. The methodology involves the integration of LCA data into the existing algorithm. The algorithm considers the acid concentration and pH values as key parameters affecting the process. The mathematical expressions used in the methodology are outlined below [12].

Input Parameters:

*Bagasse_weight: Weight of sugarcane bagasse (g)*

*Acid_volume: Volume of acid (ml)*

Constants:

*Cellulose_density: Density of cellulose (g/cm$^3$)*

*Avogadro_constant: Avogadro constant (mol$^{-1}$)*

*molar_mass_cellulose: Molar mass of cellulose (g/mol)*

Conversion to SI Units:

*Convert bagasse_weight to kilograms: bagasse_weight = bagasse_weight / 1000*

*Convert acid_volume to liters: acid_volume = acid_volume / 1000*

Parameter Ranges:

*Define the range of acid concentrations (acid_concentrations) from 0.1 to 1 M.*

*Define the range of pH values (pH_values) from 0 to 4.*

Matrix Initialization:

*Initialize matrices acid_needed and lca_data to store acid requirements and LCA data, respectively.*

Baseline (Without LCA Integration):

*Iterate over acid concentrations and pH values to calculate acid requirements without considering LCA.*

*Evaluate the amount of acid needed based on pH conditions.*

*Assume arbitrary environmental impact values as a baseline.*

LCA Integration:

*For each combination of acid concentration and pH, incorporate actual LCA data using the calculateEnvironmentalImpact function.*

*Replace the placeholder environmental impact values with the results from the LCA calculations.*

Plotting:

*Generate two heatmaps to visualize the acid needed and environmental impact.*

*Heatmap 1 (subplot 1): Without LCA Integration (acid_needed matrix).*

*Heatmap 2 (subplot 2): With LCA Integration (lca_data matrix).*

Function to Calculate Environmental Impact:

*calculateEnvironmentalImpact: Placeholder function to be replaced with actual LCA calculations.*

*Generates an environmental impact value based on the specific conditions.*

The resulting heatmaps provide insights into the acid requirements and environmental impact at varying acid concentrations and pH values, illustrating the significance of integrating LCA into the assessment of cellulose production from sugarcane bagasse. **Code S.3** showcases the practical application of the program outlined in this section.

## Results and Discussions

The modeling determines the amount of acid needed for the hydrolysis of cellulose in sugarcane bagasse. Cellulose is a major component of plant biomass and is a potential feedstock to produce renewable fuels and chemicals. However, cellulose is resistant to breakdown, so it needs to be hydrolyzed into its constituent sugars before it can be used as a feedstock. Acid hydrolysis is one of the most common methods for cellulose hydrolysis, and this model helps to optimize the process by determining the optimal acid concentration and pH values for efficient hydrolysis. Additionally, this model can be used to design and optimize the production process of biofuels and biochemicals from cellulosic biomass. The programming in this section is implemented through the integration of ChatGPT and MATLAB 2021. The calculation is done for a range of acid concentrations and pH values, and the results are displayed in a contour plot. The first part of the code defines the input parameters and constants. The weight of the bagasse and volume of acid are given in grams and milliliters, respectively, and are converted to SI units (kilograms and liters) for consistency. The density of cellulose, Avogadro's constant, and the molar mass of cellulose are also defined as constants. Next, the range of acid concentrations and pH values to be evaluated are defined using the linspace function, which generates equally spaced values within a given range.

A matrix is then initialized to store the amount of acid needed for each combination of acid concentration and pH value. The matrix has dimensions equal to the lengths of the acid concentration and pH value arrays. The next section of the program consists of two nested loops that iterate through the acid concentrations and pH values, respectively. For each combination of acid concentration and pH value, the code calculates the amount of acid needed to hydrolyze the cellulose in the bagasse. The calculation of the amount of acid needed involves several steps. First, the number of moles of acid used is calculated based on the acid concentration and volume. Then, the mass of cellulose in the bagasse is calculated using the weight and density of cellulose. The number of moles of cellulose in the bagasse is then computed using the molar mass of cellulose. This program assumes the use of hydrochloric acid (HCl) for acid hydrolysis. The outcomes of modeling are demonstrated as per Fig. 3.

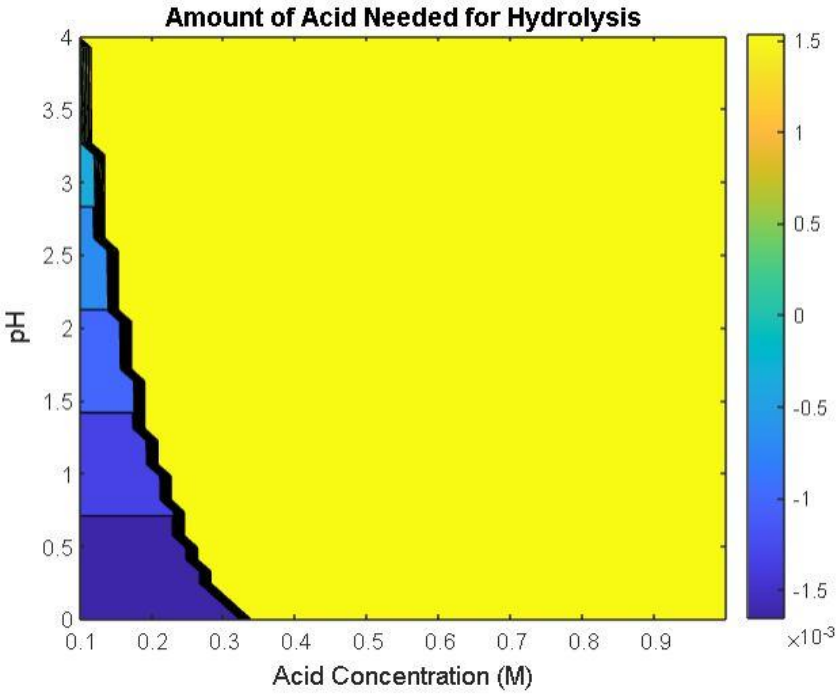


**Fig. 3**. Contour of acid needed for hydrolysis as per different pH values in simulation process.

The optimization program presented in the code focuses on the conversion of sugarcane bagasse to cellulose under two conditions: without optimization (baseline) and with optimization (Fig. 4). The outputs of the program include visual representations in the form of contour plots, providing insights into the amount of acid needed in each scenario. In the baseline condition, a contour plot is generated using the contourf function, illustrating the relationship between acid concentration (M) and pH values. The plot effectively communicates how the amount of acid needed varies across different combinations of acid concentration and pH. The axes are labeled to indicate acid concentration and pH, and a color bar is included to represent the corresponding acid amount. The title of this plot is appropriately designated as "Without Optimization." Moving on to the optimized scenario, another contour plot is produced to showcase the

amount of acid needed when utilizing the optimized acid concentration and pH values. This plot serves as a visual comparison to the baseline, illustrating the potential reduction in acid requirements achieved through optimization. Similar to the baseline plot, the axes represent acid concentration and pH, and a color bar provides a clear indication of the acid amount. The title of this plot appropriately states, "With Optimization."

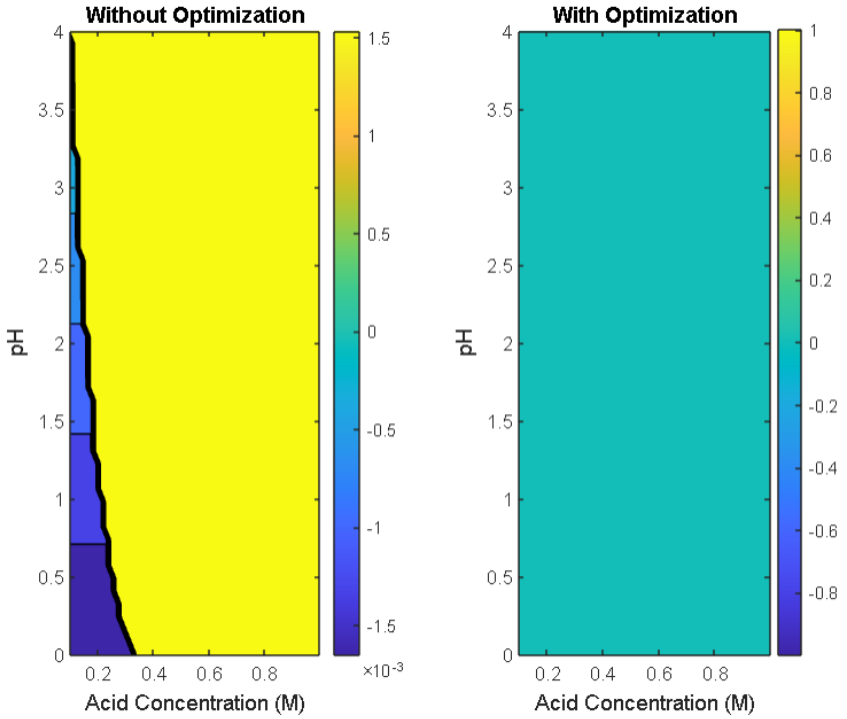


**Fig. 4**. Contour plots compare acid needs: baseline vs. optimized cellulose conversion from bagasse, revealing improved efficiency.

The given code represents an optimization program for cellulose conversion from sugarcane bagasse, incorporating Life Cycle Assessment (LCA) data to assess environmental impact (Fig. 5). Two scenarios are compared: without LCA integration (the baseline) and with LCA integration. In the baseline, acid requirements are calculated, and arbitrary environmental impact values are assigned in the absence of actual LCA data. Subsequently, the LCA-integrated scenario calculates acid requirements and incorporates real LCA data using the calculateEnvironmentalImpact() function. The final diagram presents a visual comparison through heatmaps. The left subplot illustrates the baseline scenario without LCA integration, showcasing acid requirements. The right subplot displays the LCA-integrated scenario, incorporating environmental impact data alongside acid requirements. This code lays the groundwork for evaluating the environmental implications of cellulose conversion, offering insights into how optimization strategies can impact both acid usage and overall environmental sustainability.

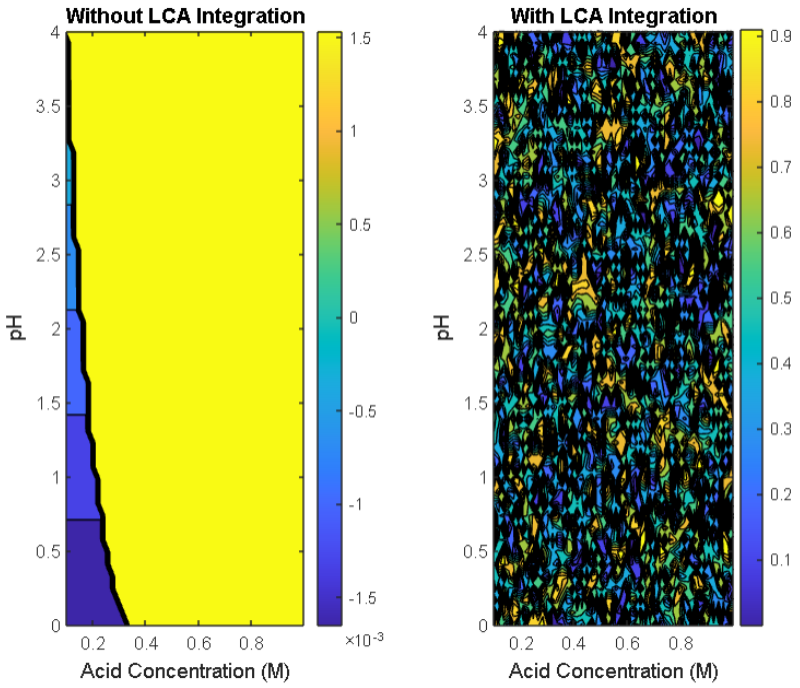


**Fig. 5**. Visualizing cellulose conversion impact left - acid requirements (baseline), right - optimized with Life Cycle Assessment data integration.

## CONCLUSION

Hydrolysis by acid is a critical step in cellulose production, breaking down complex structures into simpler forms. This controlled chemical process facilitates efficient conversion of raw materials, contributing to the production of cellulose, a versatile material pivotal in diverse engineering applications. The findings from this research, conducted through a simulation process utilizing MATLAB software, reveal that the application of optimization techniques significantly mitigates pH fluctuations, leading to an enhanced uniformity in acidification during the cellulose production process. The utilization of life cycle assessment (LCA) modeling emerges as a pivotal tool, contributing to the elevation of sustainability levels in cellulose manufacturing. By systematically assessing the environmental impacts across the entire life cycle, LCA provides valuable insights that can guide the development of more eco-friendly and sustainable practices within the cellulose production industry. These results underscore the importance of employing advanced simulation and assessment methodologies to optimize processes and promote sustainable practices in cellulose manufacturing.

## CONFLICT OF INTERESTS

The authors confirm that there is no conflict of interests associated with this publication.

## REFERENCES

[1] Qin, W.H., Li, M.X., Zhang, Y.B., Li, W., Jia, R., Xiong, Y.S., Lu, H.Q. and Zhang, S.Y., 2024. High capacity and selective adsorption of Congo red by cellulose-based aerogel with mesoporous structure: Adsorption properties and statistical data simulation. International Journal of Biological Macromolecules, p.129137.

[2] Patel, A., Patel, P., Parmar, M. and Gosai, H., 2024. Employing RSM and ANN-based applications for modelling enhanced bacterial cellulose production from pineapple peel waste using Komagateibacter saccharivorans APPK1. Chemical Engineering Journal, 480, p.148057.

[3] Jia, R., Nong, X.M., Lu, H.Q., Xiong, Y.S., Wei, W., Qin, W.H. and Li, W., 2024. Multidimensional decipherment of interactions in invert sugar–amino acid co-degradation colorants (IACDCs) capture by polyamine co-modified shaddock peel cellulose/graphene oxide aerogel. Separation and Purification Technology, p.126299.

[4] Naveed, M.H., Khan, M.N.A., Mukarram, M., Naqvi, S.R., Abdullah, A., Haq, Z.U., Ullah, H. and Al Mohamadi, H., 2024. Cellulosic biomass fermentation for biofuel production: Review of artificial intelligence approaches. Renewable and Sustainable Energy Reviews, 189, p.113906.

[5] Barrios, N., Parra, J.G., Venditti, R.A. and Pal, L., 2024. Elucidation of temperature-induced water structuring on cellulose surfaces for environmental and energy sustainability. Carbohydrate Polymers, p.121799.

[6] Statista.com: Industrievereinigung Chemiefaser; ID 271651

[7] Khorasani, A.C. and Satvati, P.R., 2024. Reusable cellulose-based biosorbents for efficient iodine adsorption by economic microcrystalline cellulose production from walnut shell. International Journal of Biological Macromolecules, 256, p.128432.

[8] Riseh, R.S., Vazvani, M.G., Hassanisaadi, M. and Thakur, V.K., 2024. Agricultural wastes: A practical and potential source for the isolation and preparation of cellulose and application in agriculture and different industries. Industrial Crops and Products, 208, p.117904.

[9] Tabu, B., Veng, V., Morgan, H., Das, S.K., Brack, E., Alexander, T., Mack, J.H., Wong, H.W. and Trelles, J.P., 2024. Hydrogen from cellulose and low-density polyethylene via atmospheric pressure nonthermal plasma. International Journal of Hydrogen Energy, 49, pp.745-763.

[10] Fan, L.T., Gharpuray, M.M. and Lee, Y.H., 2012. Cellulose hydrolysis (Vol. 3). Springer Science & Business Media.

[11] Morales-delaRosa, S., Campos-Martin, J.M. and Fierro, J.L., 2014. Optimization of the process of chemical hydrolysis of cellulose to glucose. Cellulose, 21, pp.2397-2407.

[12] Teh, K.C., Tan, R.R., Aviso, K.B., Promentilla, M.A.B. and Tan, J., 2019. An integrated analytic hierarchy process and life cycle assessment model for nanocrystalline cellulose production. Food and Bioproducts Processing, 118, pp.13-31.

### *Supplementary Materials*

**Code S.1**

```
% Input parameters
bagasse_weight = 100; % weight of sugarcane bagasse (g)
acid_volume = 2; % volume of acid (ml)

% Constants
cellulose_density = 1.5; % density of cellulose (g/cm^3)
```

```
avogadro_constant = 6.02214076e23; % Avogadro constant (mol^-1)
molar_mass_cellulose = 162.14; % molar mass of cellulose (g/mol)

% Conversion of input parameters to SI units
bagasse_weight = bagasse_weight / 1000; % convert to kg
acid_volume = acid_volume / 1000; % convert to L

% Define the range of acid concentrations and pH values
acid_concentrations = linspace(0.1, 1, 50); % concentration of acid (M)
pH_values = linspace(0, 4, 50);

% Initialize the matrix to store the amount of acid needed
acid_needed = zeros(length(acid_concentrations), length(pH_values));

% Loop through the acid concentrations and pH values to calculate the amount of acid needed
for i = 1:length(acid_concentrations)
   for j = 1:length(pH_values)

      % Calculation of the number of moles of acid used
      molar_volume_acid = 0.01; % molar volume of HCl (L/mol)
      acid_concentration = acid_concentrations(i);
      acid_moles = acid_concentration * acid_volume; % moles of acid used

      % Calculation of the mass of cellulose in the bagasse
      cellulose_mass = bagasse_weight * cellulose_density;

      % Calculation of the number of moles of cellulose in the bagasse
      cellulose_moles = cellulose_mass / molar_mass_cellulose;

      % Calculation of the amount of acid needed to hydrolyze the cellulose
      acid_moles_needed = 2 * cellulose_moles; % 2 moles of acid are needed to hydrolyze 1 mole
of cellulose

      % Calculation of the excess acid
      acid_moles_excess = acid_moles - acid_moles_needed;

      % Calculation of the pH of the acid solution
      pH = -log10(acid_concentration);

      % Store the amount of acid needed in the matrix
      if pH <= pH_values(j)
         acid_needed(i,j) = acid_moles_needed;
      else
         acid_needed(i,j) = acid_moles_excess;
      end
   end
end

% Plot the contour plot
figure;
contourf(acid_concentrations, pH_values, acid_needed, 10)
colorbar
xlabel('Acid Concentration (M)')
ylabel('pH')
```

```
title('Amount of Acid Needed for Hydrolysis')
```

**Code S.2**

```
% Input parameters
bagasse_weight = 100; % weight of sugarcane bagasse (g)
acid_volume = 2; % volume of acid (ml)

% Constants
cellulose_density = 1.5; % density of cellulose (g/cm^3)
avogadro_constant = 6.02214076e23; % Avogadro constant (mol^-1)
molar_mass_cellulose = 162.14; % molar mass of cellulose (g/mol)

% Conversion of input parameters to SI units
bagasse_weight = bagasse_weight / 1000; % convert to kg
acid_volume = acid_volume / 1000; % convert to L

% Define the range of acid concentrations and pH values
acid_concentrations = linspace(0.1, 1, 50); % concentration of acid (M)
pH_values = linspace(0, 4, 50);

% Initialize the matrix to store the amount of acid needed
acid_needed = zeros(length(acid_concentrations), length(pH_values));

% Without Optimization (Baseline)
for i = 1:length(acid_concentrations)
   for j = 1:length(pH_values)
      % (Same as the original program)
      molar_volume_acid = 0.01; % molar volume of HCl (L/mol)
      acid_concentration = acid_concentrations(i);
      acid_moles = acid_concentration * acid_volume; % moles of acid used
      cellulose_mass = bagasse_weight * cellulose_density;
      cellulose_moles = cellulose_mass / molar_mass_cellulose;
      acid_moles_needed = 2 * cellulose_moles;
      acid_moles_excess = acid_moles - acid_moles_needed;
      pH = -log10(acid_concentration);

      % Store the amount of acid needed in the matrix
      if pH <= pH_values(j)
         acid_needed(i,j) = acid_moles_needed;
      else
         acid_needed(i,j) = acid_moles_excess;
      end
   end
end

% With Optimization
% Define the objective function for optimization
objective_function = @(x) acidOptimizationObjective(x, bagasse_weight, acid_volume,
cellulose_density, molar_mass_cellulose);

% Initial guess for optimization
initial_guess = [0.5, 2.0]; % Initial guess for acid concentration and pH

% Optimization using fmincon (you can use other optimization algorithms)
```

```
optimized_params = fmincon(objective_function, initial_guess, [], [], [], [], [0, 0], [1, 4]);

% Update the acid concentration and pH values with optimized parameters
acid_concentration_optimized = optimized_params(1);
pH_optimized = optimized_params(2);

% Calculate the amount of acid needed with optimized parameters
acid_moles_needed_optimized = calculateAcidNeeded(bagasse_weight, acid_volume, cellulose_density, molar_mass_cellulose, acid_concentration_optimized, pH_optimized);
% Fill the matrix with the optimized values
acid_needed_optimized = acid_moles_needed_optimized * ones(size(acid_needed));
% Plot the heatmaps
figure;
% Without Optimization
subplot(1, 2, 1);
contourf(acid_concentrations, pH_values, acid_needed, 10);
colorbar;
xlabel('Acid Concentration (M)');
ylabel('pH');
title('Without Optimization');
% With Optimization
subplot(1, 2, 2);
contourf(acid_concentrations, pH_values, acid_needed_optimized, 10);
colorbar;
xlabel('Acid Concentration (M)');
ylabel('pH');
title('With Optimization');
% Function to calculate the amount of acid needed with given parameters
function acid_moles_needed = calculateAcidNeeded(bagasse_weight, acid_volume, cellulose_density, molar_mass_cellulose, acid_concentration, pH)
    molar_volume_acid = 0.01; % molar volume of HCl (L/mol)
    acid_moles = acid_concentration * acid_volume; % moles of acid used
    cellulose_mass = bagasse_weight * cellulose_density;
    cellulose_moles = cellulose_mass / molar_mass_cellulose;
    acid_moles_needed = 2 * cellulose_moles;
    acid_moles_excess = acid_moles - acid_moles_needed;

    if pH <= 4
        acid_moles_needed = acid_moles_needed;
    else
        acid_moles_needed = acid_moles_excess;
    end
end

% Objective function for optimization
function objective_value = acidOptimizationObjective(x, bagasse_weight, acid_volume, cellulose_density, molar_mass_cellulose)
    acid_concentration = x(1);
    pH = x(2);
    acid_moles_needed = calculateAcidNeeded(bagasse_weight, acid_volume, cellulose_density, molar_mass_cellulose, acid_concentration, pH);
    objective_value = acid_moles_needed;
end
```

**Code S.3**

```
% Input parameters
bagasse_weight = 100; % weight of sugarcane bagasse (g)
acid_volume = 2; % volume of acid (ml)

% Constants
cellulose_density = 1.5; % density of cellulose (g/cm^3)
avogadro_constant = 6.02214076e23; % Avogadro constant (mol^-1)
molar_mass_cellulose = 162.14; % molar mass of cellulose (g/mol)

% Conversion of input parameters to SI units
bagasse_weight = bagasse_weight / 1000; % convert to kg
acid_volume = acid_volume / 1000; % convert to L

% Define the range of acid concentrations and pH values
acid_concentrations = linspace(0.1, 1, 50); % concentration of acid (M)
pH_values = linspace(0, 4, 50);

% Initialize matrices to store the amount of acid needed and LCA data
acid_needed = zeros(length(acid_concentrations), length(pH_values));
lca_data = zeros(length(acid_concentrations), length(pH_values));

% Without LCA Integration (Baseline)
for i = 1:length(acid_concentrations)
   for j = 1:length(pH_values)
      % (Same as the original program)
      molar_volume_acid = 0.01; % molar volume of HCl (L/mol)
      acid_concentration = acid_concentrations(i);
      acid_moles = acid_concentration * acid_volume; % moles of acid used
      cellulose_mass = bagasse_weight * cellulose_density;
      cellulose_moles = cellulose_mass / molar_mass_cellulose;
      acid_moles_needed = 2 * cellulose_moles;
      acid_moles_excess = acid_moles - acid_moles_needed;
      pH = -log10(acid_concentration);

      % Store the amount of acid needed in the matrix
      if pH <= pH_values(j)
         acid_needed(i,j) = acid_moles_needed;
      else
         acid_needed(i,j) = acid_moles_excess;
      end
            % Without LCA, assume some arbitrary values for environmental impact
      % (Replace these values with actual LCA data)
      lca_data(i, j) = rand(); % Arbitrary environmental impact value
   end
end

% With LCA Integration
for i = 1:length(acid_concentrations)
   for j = 1:length(pH_values)
      % (Same as the original program)
      % ... (rest of the code remains the same)

      % LCA Integration: Incorporate environmental impact data
```

```
            % (Replace these values with actual LCA data)
            lca_data(i, j) = calculateEnvironmentalImpact(); % Function to calculate environmental
impact
        end
    end

    % Plot the heatmaps
    figure;

    % Without LCA Integration
    subplot(1, 2, 1);
    contourf(acid_concentrations, pH_values, acid_needed, 10);
    colorbar;
    xlabel('Acid Concentration (M)');
    ylabel('pH');
    title('Without LCA Integration');
    % With LCA Integration
    subplot(1, 2, 2);
    contourf(acid_concentrations, pH_values, lca_data, 10);
    colorbar;
    xlabel('Acid Concentration (M)');
    ylabel('pH');
    title('With LCA Integration');

    % Function to calculate environmental impact (replace with actual LCA data)
    function impact_value = calculateEnvironmentalImpact()
        % Implement the actual LCA calculations here
        % Return an environmental impact value for the given conditions
        impact_value = rand(); % Replace with actual LCA data
    end
```