Biobutanol and bioethanol production from agricultural wastes: A cell phone application for computing the bioconversion rates

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Abstract: To carry out the calculations required for modelling and computing for kinetics biobutanol and bioethanol yields and production rates, several procedures should be accomplished; this requires time and effort, and there is a chance that mistakes will be made. The goal of this study is to provide a tool that will assist users, engineers, and experts in conducting these computations by creating a mobile application to reduce time and effort. The calculations were carried out using a mathematical model. The mathematical model was then included in a flowchart that was created later. After that, Kodular was used to configure the mobile application by fusing the interface design, mathematical model, and flowchart. Information was gathered from publications, wastewater treatment facilities, non-governmental organizations (NGOs), and government groups. To offer output data that matched the output data obtained from the configured program, the data collected for doing the calculations in the conventional manner was used. Both the standard strategy and the program's outcomes were consistent. The created mobile application can do kinetic modeling and determine the yields and rates of generation of biobutanol and bioethanol from agricultural waste.

Keywords: Biobutanol, bioethanol, software program, a mobile application, agricultural wastes.

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1Introduction

Increased petroleum costs and the depletion of fossil resources are the primary drivers behind the global quest for alternative energy resources (Abdelsalam et al., 2021). Besides, environmental concerns and issues have been raised regarding emissions of greenhouse gases (Alengebawy et al.,

2022; Samer et al., 2014). Researchers are becoming more interested in the bioconversion of biomass and agricultural wastes into alcoholic fuels, including bioethanol (C_2H_5OH) and biobutanol (C_4H_9OH) (Nimbalkar et al., 2018; Attia et al., 2022; Saeed et al., 2022). Alcohols generated biologically are gaining popularity as liquid transportation fuels and renewable solvents (Karthick and Nanthagopal, 2021; Shanmugam et al., 2021). According to market research, the value of biochemicals and products would surpass \$23 billion by 2025 (Shanmugam et al., 2021). Although bioethanol is currently mass-produced, biobutanol offers enhanced fuel properties as well as

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extra use as a chemical precursor and solvent (Dehghanzad et al., 2020). Biobutanol also offers a higher energy density, could be utilized in larger mix ratios, and is therefore more suitable for the existing transportation infrastructure (Keller et al., 2015; Meramo-Hurtado et al., 2020; Shanmugam et al., 2021). Various agricultural wastes have been utilized as supply for the production of biobutanol and bioethanol, including rice straw, wheat straw, corn stover, and sugarcane bagasse, etc. (Karthick and Nanthagopal, 2021; Nimbalkar et al., 2018; Procentese et al., 2017; Saeed et al., 2022).

Biobutanol and bioethanol synthesis from biomass wastes not only provides a sustainable green energy source, but also has the potential to mitigate greenhouse gas effects and global warming to a large extent (Huzir et al., 2018; Rathour et al., 2018; Samer, 2022). However, there are several calculations and procedures (e.g., enzymatic saccharification rate, acetone-butanol-ethanol (ABE) conversion rate, bioconversion rate, etc.) that should be accomplished for the production of biobutanol and bioethanol (Gao and Rehmann, 2014; Nimbalkar et al., 2018), which consume significant time and efforts and could also trigger major errors that affect products quality. Researchers and policymakers across the world have emphasized the importance of devolving cell phone applications to support specialists and farmers in developing countries (Bateki et al., 2021), and thereby enhance their livelihood and ensure energy security. There is rising confidence that applications of information and communication technology (ICT) could improve food and energy security in developing countries (Bateki et al., 2021). Thus, it is essential to develop a tool (i.e., cell phone application) to support specialists, policymakers, engineers, and other users in conducting these computations to save their time and efforts and eliminate any potential mistakes.

A software program is a smart computer program that resolves problems logically. It is difficult to solve

and require a high level of skills to resolve. Those software products use heuristics and symbolic interpretations of scenarios to mimic experts' logical thinking. An artificial intelligence and information technology engineer's main objective is to record the heuristics and/or reasoning patterns used by specialists in the execution of complicated problem-solving tasks and present them in the design of electronic spark maps (i.e., decision trees) (Samer et al., 2019, 2011). Software applications perform a wide range of tasks; operational classifications for software systems include prediction, interpretation, instruction, diagnosis, debugging, monitoring, repair, control, planning, and design (Raj et al., 2021; Samer et al., 2013, 2022). Hybrid systems are created by combining mathematical models with software applications. The advantages of hybrid systems include the ability of computations to provide quantifiable data to software, that in turn provides important inputs for simulation studies (Samer et al., 2012, 2013). A software application has the traditional structure of a computer software that uses equations and/or rules to interpret data or information input by the user certain issues (Samer, 2010; Samer et al., 2019). Several smart phone applications have been created to aid policymakers and farmers in developing countries reduce socio-economic constraints and enhance supply chain management. However, most of the studies are mainly focused on crop and animal production (Bateki et al., 2021; Baumüller, 2018; Eitzinger et al., 2019; Ngugi et al., 2020).

To the best of our knowledge, no published studies have developed a user-friendly cell phone application that can be used for computing the production rates and yields of biobutanol and bioethanol. Thus, this study aims to create a user-friendly cell phone application that will assist engineers, specialists, policymakers, and various users in conducting various computations to save their efforts and time and eliminate any potential mistakes. Specifically, the application aims to perform kinetic modeling and compute biobutanol and bioethanol yields and production rates.

2 Materials and methods

2.1 Gaining information

The parameters, constants, variables, and factors of the simulation models were used to produce the biobutanol and bioethanol available production units from the references (Gao and Rehmann, 2014; Kang et al., 2015; Sasaki et al., 2014). In order to duplicate their expertise thinking and use it in constructing the organized induction of the mobile application, communications were also established with specialists in the following Egyptian institutions:

- 1. Ministry of Environment and Egyptian Environmental Affairs Agency
- 2. Ministry of Agriculture and Land Reclamation
- 3. Agricultural Research Center
- 4. New and Renewable Energy Authority

5. Corporation of Bioenergy for Sustainable Rural Development

6. Biobutanol and bioethanol lab-scale production systems

Having gathered a vast number of facts and knowledge information, a software that can be installed on mobile devices was created to assist users, engineers,

and experts in computing the performance variables, factors, and parameters of biobutanol and bioethanol production. The program is made to carry out kinetic modeling and compute the biobutanol and bioethanol yields and production rates. Therefore, this software is an intelligent system that applies knowledge, reasoning, and rational processes to resolve complex problems for which finding a solution requires a great deal of experience. This software manipulates heuristics and symbolic representations of knowledge to imitate the thought processes of experts. Hybrid systems are created by combining mathematical models and software programs. Mockups provide qualitative and quantitative data for the software, which in turn provides missing parameters for the simulation models, which is a benefit of hybrid systems.

2.2 Data acquisition

The aforementioned institutions provided the data used to configure the software. The data that were collected and used to validate and assess the software program that was produced are displayed in Tables 1 and 2. The output data, or calculated data, are represented by the gray-highlighted columns. The input data is represented by the remaining, unhighlighted columns.

Biobuta nol lab-scale producti on system	Amount of Starch Cellulose and Hemicellul ose Contained in each Substrate (g)	Amoun t of Glucos e Produc ed (g)	Enzymatic Saccharificat ion Rate (%)	Amoun t of ABE Produc ed (g)	Theoreti cal Maximu m Amount of ABE Produce d	ABE Conversi on Rate (%)	Maximum ABE Concentrat ion (g L ⁻¹)	Fermentat ion Time (h)	Overall Producti on Rate (g L ⁻¹ h ⁻ ¹)	ABE Concentrat ion (g L ⁻¹)	Substra te Volum e (L)	AB E Yiel d (g)
1	188	95	45.48	35		51.43	35		0.486	35	1	35
2	225	133	53.20	29	0.362 g of ABE	60.23	29		0.403	29	3	87
3	153	77	45.29	15	from 1 g	53.81	15	72	0.208	15	5	75
4	211	109	46.49	22	of Glucose	55.76	22		0.306	22	3	66
5	279	151	48.71	31		56.71	31		0.431	31	2	62

Table 1 Data of biobutanol lab-scale production systems

49.67

42.04

49.33

47.09

1.316

0.880

1.367

1.069

Purificatio n Process Efficiency (%)

80.62

74.92

76.71

81.41

81.85

			Table 2 I	Jala of I	Joethanoi lab	-scale product	ion systems		
Bioethanol lab-scale production system	Initial Dry Biomass Concentration (g L ⁻¹)	Cellulo se Fractio n of Dry Biomas s	Total Bioethanol Produced (g L ⁻¹)	Bioet hanol Yield (%)	Theoretical Ethanol Concentration (g L ⁻¹)	Ethanol Produced Concentration (g L ⁻¹)	Bioconversi on Rate (%)	Volume of Partially Purified Ethanol in Distillate (mL L ⁻¹)	Crude Ethanol in Fermentation Broth (mL L ⁻¹)
1	19		1.235	28.63	2.985	1.235	41.37	0.786	0.975

3.356

2.652

3.511

2.877

1.667

1.115

1.732

1.355

Table 2 Data of bioathanol lab-scale production systems

21 2.3 Mathematical modeling

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17

28

2.3.1 Biobutanol calculations

2.3.1.1 Enzymatic saccharification rate

The enzymatic saccharification rate will be calculated as follows (Sasaki et al., 2014):

0.4

1.667

1.115

1.732

1.355

29.36

28.88

27.23

28.41

Enzymatic saccharification rate (%)=

(Amount of glucose produced (g))

(Amount of starch or cellulose and hemicellose contained in each substrate (0.9(g))

(1)

2.3.1.2 ABE conversion rate

The acetone-butanol-ethanol (ABE) conversion rate will be calculated as follows (Sasaki et al., 2014):

ABE conversion rate(%) =(amount of ABE produced) (theoretical maximum amount of ABE produced (0.362g of ABE from 1 g of glucose))

(2)

2.3.1.3 Overall ABE production rate

The overall output production rate (g L⁻¹ h⁻¹) will be calculated as the highest acetone-butanol-ethanol (ABE) concentration achieved (g L^{-1}) divided by the fermentation time (h). ABE Yield (g) will be calculated as the ABE concentration (g L⁻¹) in the fermented substrate multiplied by the volume of the fermented liquid substrate (L), where these calculations will be conducted as follows (Gao and Rehmann, 2014):

Overall production $rate(gL^{-1}h^{-1}) = \frac{Maximum ABE \ concentration(gL^{-1})}{Fermentation \ time(h)}$ (3)

ABE Yield (g) = ABE Concentration $(g L^{-1}) \times Substrate Volume(L)$ (4)

2.3.2 Bioethanol calculations

2.3.2.1 Bioethanol yield

The bioethanol yield (%) will be calculated as

follows (Kang et al., 2015; Singhania et al., 2014):

0.986

0.675

1.113

0.875

$$Ethanol \ yield 0 = \left\lfloor \frac{\left[\left(EtOH_f - EtOH_0\right)\right]}{0.511 * \left[Biomass\right]_0 * 1.111} \right\rfloor * 100\%$$
(5)

where, $\{EtOH_f - EtOH_0\}$ indicates total bioethanol resulting from fermentation (g L^{-1}) run, [Biomass]₀ is the initial concentration of dry biomass (g L^{-1}), f is dry biomass's cellulose fraction, 0.511 is the rate of conversion of glucose to bioethanol based on the stoichiometric yeast biochemistry and 1.111 is the cellulose to equivalent glucose conversion factor.

2.3.2.2 Bioconversion rate

The bioconversion rate (%) will be determined as following (Khuong et al., 2014):

 $Conversion \ rate(\%) = \frac{Ethanol \ produced \ concentration \ g \ L^{-1}}{Theoretical \ ethanol \ concentration \ g \ L^{-1}} \times 100$

(6) The theoretical bioethanol concentration (g L^{-1}) will be calculated as follows (Khuong et al., 2014):

Theoretical ethanol concentration $gL_{-1} =$ Glucan concentration $\times 1.0 \times 0.51 + Xylan$ concentration $\times 1.14 \times 0.46$ (7)

Where, 1.11 is the glucose-derived from-glucan conversion factor, 1.14 is the xylose-derived fromxylan coefficient (Sluiter et al., 2008); 0.51 is the rate at which ethanol is produced from glucose, and 0.46 is ethanol produced from xylose at a certain coefficient (Aita et al., 2011).

2.3.2.3 Purification process efficiency

process of purifying effectiveness of The bioethanol obtained by distillation will be determined using the subsequent equation (Das et al., 2013; Gupta et al., 2014):

2

3

4

5

(8)

purification process efficiency (%) =

 $\frac{(volume of partially purified ethanol in distillate (mL / L))}{(crude ethanol in fermentation broth (mL / L))} \times 100$

2.4 Authentication and valuation

Finding out whether a piece of software is functioning properly is the goal of its authentication.

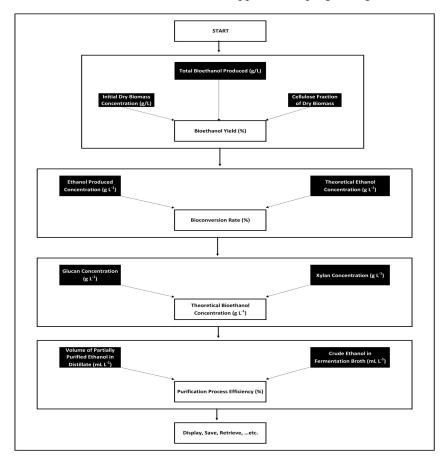
Additionally, evaluating software seeks to establish the program's accuracy. The taught data were used to do computations using the normal method to obtain the output data, which were then compared to the output data shown by the program. The program's output data and that of the traditional way would be comparable.2.5 Programming languages

2.5 Programming languages

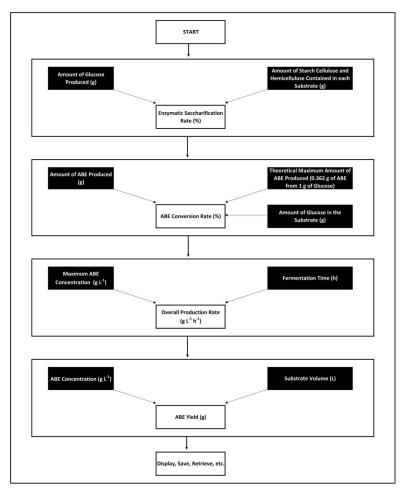
Kodular is a web application integrated development environment. It features a graphical user interface (GUI) similar to the StarLogo and Scratch programming languages, which supports operators in dragging and dropping visual objects to make an application that is able to operate on android-supported cell phones with Kodular Companion, which is the software that supports the cell phone application to run and debug on.

2.6 Programming

By combining the flowchart and the mathematical model and creating the user interface in Kodular, the mobile application was created. Figure 1 shows the diagrams that illustrate the adopted measures to run the application, where (a) is the diagram of biobutanol and (b) is the diagram of bioethanol. The programmed software is comprised of six programming nodes and is configured into 11 codes. Figures 2 and 3 show examples of the programming nodes. Figures 4 through 12 show examples of the codes that comprise the programming syntax. On the other hand, Table 3 displays the resources that were employed in the application's programing.



(a) The diagram of biobutanol



(b) The diagram of bioethanol

Figure 1 Diagrams illustrate the adopted measures to run the application

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Figure 2 Programming node 1

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Figure 3 Programming node 2

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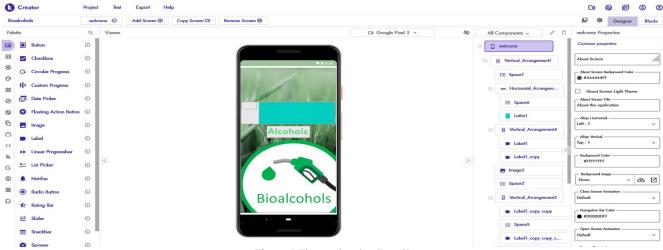


Figure 5 The used codes (Part 2)

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Figure 8 The used codes (Part 5)

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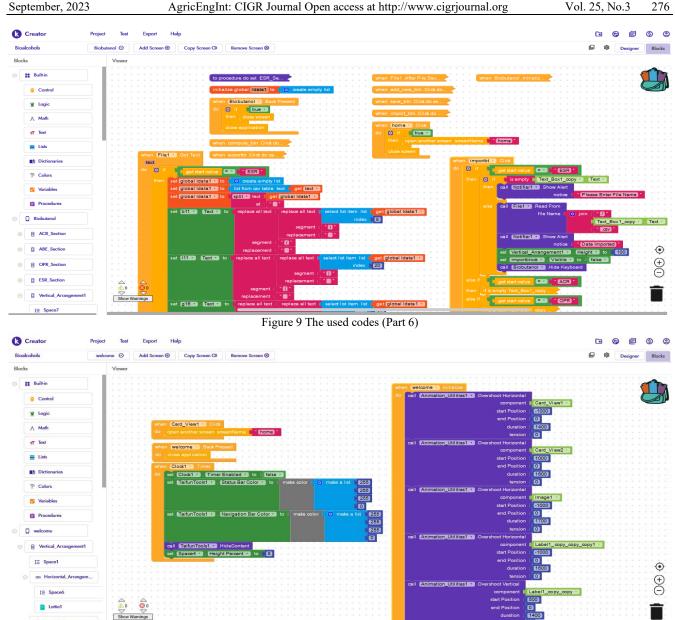


Figure 10 The used codes (Part 7)

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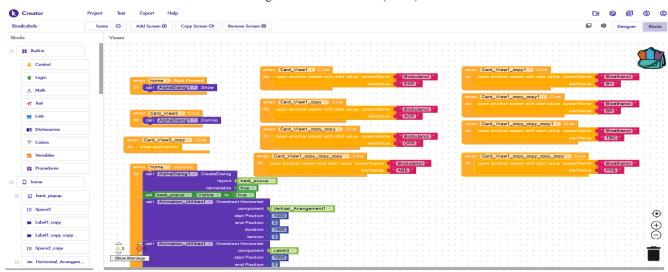
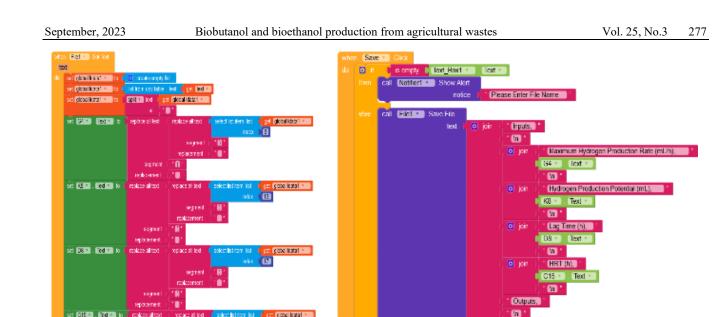


Figure 11 The used codes (Part 8)



Tools	Types and Importance
Add New	Adding new data set
Import	Load data from CSV file
Compute	Compute data and get results
Save	Export data and save in CVS file for later use
Home	To choose a different model, go back to the application's home screen.

Figure 12 The used codes (Part 9) Table 3 The tools that were utilized to program the application

3 Results

I GINE TOTAL

The created program is capable of performing kinetic modeling and computing the biobutanol and bioethanol yields and production rates. The simulation's outcomes are displayed in Figures 13 -21, where the figures display the data for the input and output. The software was created in such a way that when input data are provided, the results of the kinetic modeling and the yields and production rates of biobutanol and bioethanol show automatically. The figures are styled as following:

Figure 13 shows the structure of the developed application for smartphones, which contains the Splash screen, Welcome screen, and Main Screen.

Figure 14 shows the Main Screen, while Figure 15 demonstrate the mobile application's main window, where the user can choose between the biobutanol calculations or the bioethanol calculations.

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Figure 16 displays the input and output data from the modeling-related calculations of biobutanol calculations, where the user should enter the amount of cellulose and starch found in each substrate (g), and the Amount of Glucose Produced (g). Then, the application automatically computes the Enzymatic Saccharification Rate (%).

Figure 17 illustrates the input and output data from the modeling-related calculations of biobutanol calculations, in which the user must enter the values for the Amount of ABE Produced (g), and the Theoretical Maximum Amount of ABE Produced. The software then automatically determines the ABE Conversion Rate (%).

Figure 18 displays the input and output data from the modeling-related calculations of biobutanol calculations, where the user is supposed to enter data of the Maximum ABE Concentration (g L^{-1}), and the Fermentation Time (h). The software then calculates the Overall Production Rate automatically (g L^{-1} h⁻¹).

Figure 19 illuminates the input and output data from the modeling-related calculations of biobutanol calculations, in which the user must enter the values of the ABE Concentration (g L^{-1}), and the Substrate Volume (L). Then, the program computes, automatically, the ABE Yield (g).

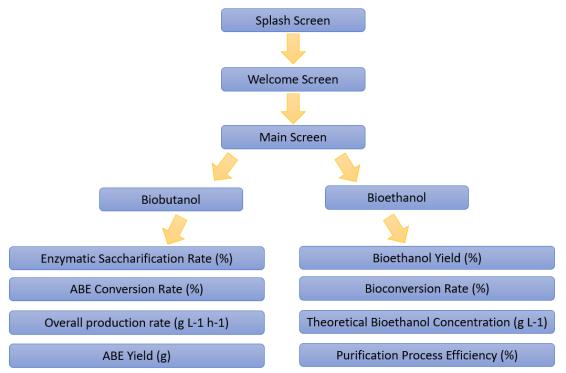
Figure 20 shows the input and output data from the modeling-related calculations of bioethanol calculations, where to enter values by the user of the Initial Concentration of Dry Biomass (g L⁻¹), the Dry

Biomass Cellulose Fraction, and the Total Bioethanol Produced (g L⁻¹). At that time, the program automatically computes the Bioethanol Yield (%).

Figure 21 demonstrates the input and output data from the modeling-related calculations of bioethanol calculations where the user is supposed to enter data of the values of the Theoretical Ethanol Concentration (g L^{-1}), and the Ethanol Produced Concentration (g L^{-1}). Hence, the software routinely computes the Bioconversion Rate (%).

Figure 22 shows the input and output data from the modeling-related calculations of bioethanol calculations, where the user should input the values of the Volume of Partially Purified Ethanol in Distillate (mL L⁻¹), and the Crude Ethanol in Fermentation Broth (mL L⁻¹). Then, the program robotically computes the Purification Process Efficiency (%).

Furthermore, the program enables the user to store computed input and output data as well as to retrieve and reprocess these data.



Bioalcohols App Structure

Figure 13 The designed mobile application's structure



Figure 14 Main screen of the cell phone application

ABE Conversion Rate (%)
INPUTS
Amount of ABE Produced (g)
A 35
Theoretical Maximum Amount of ABE Produced (0.362 g of ABE from 1 g of Glucose)
A 0.362
Amount of Glucase in the Substrate (g)
<u>A</u> 188
OUTPUT
ABE Conversion Rate (%)
A 51.42824
■ Compute ● Add New
🗄 Save 📲 Import 🎓 Home

Figure 17 Screen of ABE conversion rate calculation



Figure 20 Screen of bioethanol yield calculation

1	Velcome To BioAlcohols App
	Biobutanol Calculations
	Bioethanol Calculations

Figure 15 Input and output data screen for main window of the different models

	INPUTS	
Maximum ABE C	oncentration (g	1 L-1)
A 35		
Fermentation Tir	me (h)	
A 72		
	OUTPUT	
Overall Producti	ion Rate (g L-1 h	i-1)
A 0.48611		
		Add New
	•	
E Compute	e d -Si Import	A Home

Figure 18 Screen of overall production rate calculation



Figure 21 Screen of bioconversion rate



Figure 16 Screen of enzymatic saccharification rate calculation

INPUTS
ABE Concentration (g L-1)
<u>A</u> 35
Substrate Volume (L)
<u>A</u> 1
OUTPUT
ABE Yield (g)
A 35
☑ Compute ● Add New
🗄 Save 📲 Import 🎓 Home

Figure 19 Screen of ABE yield calculation



Figure 22 Screen of purification process efficiency calculation

4 Discussion

The obtained data were utilized to carry out calculations using the traditional technique, yielding results that were contrasted with the result information calculated by the created mobile application. The output data from the traditional method and the mobile application were identical. As a result, the mobile phone application can be used efficiently to estimate the dynamical modeling to determine the biobutanol and bioethanol yields and the production rates by using agricultural waste. The following list of advantages of the created mobile application can be provided: (1) non-professional users of the mobile application, such as students and practitioners, can use it with ease, (2) The mobile application is compact in size, and (3) The mobile application enables operational updates, (4) The mobile application is simple to download and use, and (5) students in the learning process can easily utilize the mobile application.

4.1 Programming concepts

Two different programming principles have been adopted to configure and build this cell phone application. The design technique and structured system analyses are the first programming theories that were implemented to identify the application's Specifically, technical aspects. the system configuration is broken down into sub-models, each of which has a series of phases, each of which has many actions, and each of which has a number of tasks associated with it. Subsequently, Kodular was utilized for buffering the application from components to specified functions. Kodular is a free Android app creator that offers many benefits, including a userfriendly format, graphs can be plotted for various parameters, and the software is widely supported by many devices (Syarlisjiswan et al., 2021; Mekala et al., 2021).

4.2 Structured induction

The acquisition of knowledge is acknowledged as

the cornerstone in the configuration of software. The primary task of machine learning is induction, which is the opposite of the deduction process (Mooney, 2000). Induction is a frequent method in which thorough understanding is applied to a situation in order to predict the outcome of a certain process through deducing basic principles from specific data (Mooney, 2000; Samer et al., 2019). Induction takes specific situations and generates knowledge that is aligned with these principles. Depending on a collection of inputs, rules representing a thorough understanding are derived and organized into a decision tree, which was formerly known as the spark map (Samer et al., 2013). The electronic decision tree is subsequently transformed into a necessary knowledge foundation for software configuration (Mooney, 2000). The decision tree is then able to communicate information through situations and an effective framework. The acquisition of knowledge and its conceptual model when using structured induction, an algorithm is employed to generate rules. The generated algorithm's responsive variables, coefficients, constants, and standards are then configured to serve as input-output information by the relevant decision tree for interface creation.

Structured induction applies an algorithm to a set of situations, which results in a decision tree that has been adjusted based on predefined conditions, with meaningful physical attributes choices made at terminal nodes and division nodes. The declarative data is then shaped using induction in order to decrease ambiguity of the spark map structure in terms of its degree (Samer et al., 2019). When it comes to software design, induction is a powerful machine learning technique. Induction can provide systematized information suggesting correct know-how when used utilizing some common sense in the function of the AI technologist (Samer et al., 2019, 2011). Nevertheless, induction should be viewed as one of various methods for gaining knowledge (Chaudhary et al., 2012). Whether induction is used or not, communication amongst the

artificial intelligence (AI) technologists and biofuel experts is an essential part of the process.

4.3 End users

When it comes to offering access to complex software, there is a possible downside. Users' ability to make or have judgments made for them that they did not previously have knowledge and expertise may be greatly enhanced by such developed friendly-user cell phone applications. Thus, it is expected that this developed cell phone application will benefit engineers, policymakers, students, practitioners, specialists, and non-specialists in biobutanol and bioethanol production. Additionally, the developed application can be used by professors for teaching purposes.

4.4 Educational effect

The developed application could be efficiently used in different e-module learning patterns, including phone-based training (PBT) and computer-based training (CBT), in which students complete particular instructions using their cell phones. Additionally, the application could be included in the biobutanol and bioethanol calculations assignments and problem-based learning models, in which the participants can practice using the cell phone application. A recent survey study showed that 83% of the students were satisfied with the e-module teaching models using Kodular software (Syarlisjiswan et al., 2021). The capacity of the decision-making process can be further expanded through enhancing the knowledge and expertise of the decision-makers and providing them with sufficient information for impactful decisions.

5 conclusion

This study developed a mathematical model and cell phone application to compute the biobutanol and bioethanol yields and production rates from agricultural wastes. The developed flowchart was then coupled with the algorithm, and Kodular was used to combine the flowchart and algorithm and build the user experience for the mobile phone app. To perform the computations, several data sets were gathered from wastewater treatment plants, government agencies, non-governmental organizations (NGOs), and literature. For comparison purposes, the computed output data obtained from the developed cell phone application were contrasted with the computed output data from the conventional method. The output data from both the conventional technique and the cell phone application were comparable, confirming the reliability of the developed application. As a result, the proposed program, it can be argued, might be used effectively for calculating the production rates and yields of biobutanol and bioethanol from agricultural wastes and for computing the kinetic modeling.

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