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Research Paper

Aspen Plus Simulation-based Thermodynamic Assessment of Multistage Coffee Oil Extraction from Arabica Spent Coffee Ground

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ABSTRACT*: The potential source of lipid material is spent coffee grounds (SCG). However, simultaneously, polar co-compounds (e.g., caffeine, chlorogenic acid, and cafestol) can be leached using ethanol-based processing, which must be separated in stages. The article is a thermodynamic study on an equilibrium-based multistage coffee-oil separation flowsheet with ethanol solvent (treated as 96 %(w/w) ethanol in this study) and a dry-basis definition of the feed. The flowsheet was adjusted to represent a sequential mixer-separator with solids proceeding stage-to-stage and fresh solvent contacts, with the first and second stages intended to demonstrate the leaching process, and the rest performed the purification process. Stagewise results indicate that cumulative elimination of the three monitored polar compounds is over 97% at Stage 3 and over 99.9% at Stage 4, and there is a plateau in the impurity removal; additionally, Stage 5 provides only slight further elimination. At the fifth level, oil recovery drops beyond the 69% (S/F 1:1, 40 C) to 58 (S/F 5:1, 60 °C), where an equilibrium-based trade-off between separation ability and lipid retention is shown. Varying binary interaction parameters (BIP) by 10% values resulted in slight alterations of recovery and never affected the qualitative stagewise inferences. Since this work is only done with the simulations of equilibrium, all the performance values are to be understood as the thermodynamic tendencies and the upper-bound signal; engineering design is to be suggested with an explicit experiment and with the separation/solvent-recovery studies on the laboratory level.*

Keywords: *Coffee oil, Multistage Extraction, Process simulation, Spent Coffee Grounds, Thermodynamic Assessment*

1. INTRODUCTION

Coffee is classified in the kingdom of *Plantae,* primarily spread across three different cultivated species: *Coffea arabica* (Arabica), *Coffea canephora* (Robusta), and *Coffea liberica* (Liberica) with each having its own chemical and sensory traits [1]. Among them, the Arabica coffee considered the most consumed, due its special taste and aroma, a smooth and not bitter flavor profile that suits the global specialty coffee requirements [2], [3]. In Indonesia, this coffee species mainly founded in the high-altitude areas, such as Gayo, Toraja, and Java, because of the favorable climate requirements [4]. The dominance of Arabica coffee production in Indonesia also suggests that high amounts of SCG produced inside the country are considered as Arabica species, thus affecting the SCG treatment as a waste. That is why the potential of valorization of Arabica-based SCG becomes a very valuable idea to be considered to create local sustainable processing pathways.

SCG are large-scale waste products that produced after conducting brewing and processing activities of coffee [1], [5]. Thus, the existence of SCG can be discussed as a challenge and a renewable resource in accordance with environmental factors. Considered as wastes, SCG are usually thrown into landfills, thus contributing into solid waste and greenhouse gas emissions [6]. Nevertheless, a number of investigations have shown that SCG contained about 10-20 wt.% of lipids (primarily TAG) as well as desirable phenolic compounds, thus can be used in biorefinery applications [7], [8]. Therefore, the idea of transforming SCG into

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practical products like bio-oil, bioplastics and bioenergy from its extracted oil has gained more and more interest as one of the aspects of sustainable waste management [9], [10]

The extensive production of SCG on the global level provides both environmental and economic incentives to recycle their precious parts. When not properly disposed of, SCG can give out methane when placed in an anaerobic state and can also occupy large areas of landfills [5], [11]. On the other hand, they are also abundant in carbohydrates, proteins, and most importantly lipids and thus make SCG a good raw material to extract and transform into high-value bioproducts. It has been evidenced that recovered coffee oil may be used in the cosmetics and food additives and biofuel production sectors, which generate extra income sources and decreases waste production [1], [5], [12] .

This process of extracting oil coffee out of SCG is significant specifically due to the fact that the lipid fraction of this oily product is full of valuable fatty acids that have a variety of applications. The common types of compositions that are reported in literature are linoleic acid (45-50 %(w/w)), palmitic acid (34-40% (w/w)), and oleic acid (7-10 %(w/w)) as the major constituents and minor constituents such as stearic and arachidic present in minor amounts [13], [14]. These lipids could be the sources of several applications, such as biodiesel. In addition, the process of removing coffee as soon as it is brewed is also favorable to avoid oxidation and degradation of unsaturated fatty acids that otherwise may decrease the quality of oil and limit its usage [15], [16]. Therefore, the extraction of coffee oil in SCG is in line with the principles of the circular economy and sustainable production goals.

Although the use of SCG as an oil-bearing biomass is a relatively well-investigated material, most of the existing literature uses time-dependent experimental extraction with subsequent reported yields highly dependent on particle size, agitation and contact time. This research is a thermodynamic screening model, that is ascertained to estimate maximum lipid recovery, solvent loading characteristics, and important thermodynamic sensitivities of oil-phase contact with stagewise solvent in the extraction of coffee oil with 96% (v/v) food grade ethanol. The use of Aspen Plus is not to define the extraction kinetics or even suggest an industrial flowsheet, but to offer a theoretical reference point, which can help in determination of experimental design. The results are intended to provide a thermodynamic reference that can guide solvent selection and experimental design by identifying recovery levels that are theoretically achievable prior to the consideration of mass-transfer limitations and biomass microstructure effects[17], [18].

2. MATERIAL AND METHOD

2.1. Material

The raw material used in this simulation study was Arabica SCG, which was considered as an oil-bearing biomass residue. The compositional data of Arabica SCG were adjusted based on study, as shown in Table 1, with 75 % (w/w) of the lipid consisting of TAGs [5]. These lipids were modeled as surrogates in the simulation environment, consisting of components to replicate the total composition of coffee oil, as shown in Table 2. Ethanol 96% (w/w), was used as the extraction solvent because it is a non-toxic, environment-friendly solvent and can be separated easily, as indicated in the study of [8], [19].

Table 1. SCG Composition

Component	Content (w/w)*
Protein	0.100
Lipid	0.220
Polysaccharides	0.680
*dry basis	

Table 2. Detailed Lipid Composition

Component	Content (w/w)*	Component	Content (w/w)*	Component	Content (w/w)*
TAG LLL	0.090	MAG LL	0.006	caffeine	0.002
TAG PPP	0.080	MAG PP	0.005	CGA	0.002
DAG LL	0.006	L	0.008	cafestol	0.001
DAG PP	0.005	P	0.006		

*dry basis
*chlorogenic acid (CGA)
*CGA and caffeine are assumed to have affiliation with lipids, thus consisted in the lipid fraction

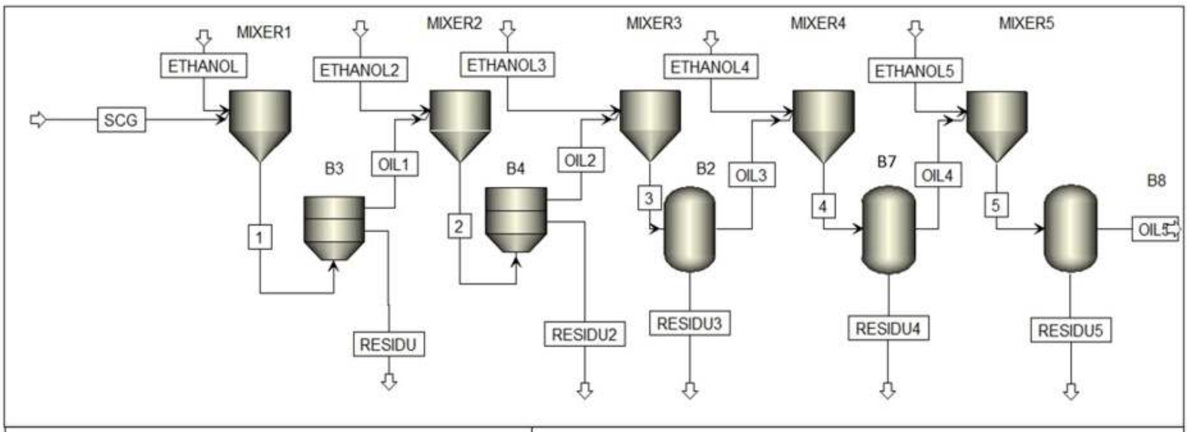
2.2. Method

2.2.1. Simulation Framework and Thermodynamic Method

Aspen Plus (Version 12.0) was used to conduct process simulations. Equilibrium assumptions were made to model the system in order to assess the stagewise separation behavior and phase partitioning. No reaction kinetics, mass-transfer coefficients, or rate-based models were included. The Non-Random Two-Liquid (NRTL) activity coefficient model was used to describe liquid-liquid equilibrium (LLE) behavior and is commonly used with non-ideal mixtures of polar solvents and complex organic compounds [12], [17], [20]. Universal Quasichemical Functional-group Activity Coefficients (UNIFAC)-Lyngby was used to estimate binary interaction parameters (BIPs), as previously used in the studies with LLE systems of lipids and bio-based compound, with polar solvents [12], [17]. In the sensitivity analysis, a systematic variation of the thermodynamic model was done by -10% and +10% of the selected BIPs as compared to their original values to assess the strength of the model. The generated BIPs are shown in **Supplementary Table 1.**

2.2.2. Multistage Separation Flowsheet and Stage Functionality

An amended multistage flowsheet was created so as to clearly differentiate between the regime of washing and separation, as shown in figure 1. The general scheme was a series of five stages in between which there were mixer-separator units that were run in steady-state. Stages 1 and 2 were referred to as leaching and washing stages. The major role of these steps was to facilitate solvent exposure on the SCG matrix, which helps to extract the easily soluble polar compounds and helps to remove the solid matrix on the liquid phase. The stages were not meant to offer any discriminatory distinction between lipids and impurities but to lessen the effects of the matrix before the downstream separation. Stages 3 5 were referred to as purification stages. LLE was the most dominant force in the separation behavior in these stages between the ethanol-rich phase and the lipid-rich phase. The stages were thus employed to assess the oil recovery and impurity removal as functions of the operating conditions. The stagewise classification was used throughout the analysis in order to prevent perplexing the efficiency of washing with equilibrium-controlled separation performance. The complete mass-stream result example, taken from S/F 2.5:1, 40°C temperature (calculated using original estimated BIP) is presented on Supplementary Table 2**.**



SCG: Spent Coffee Ground

1,2,3,4,5: Output stream of mixer

B3, B4: Solid Liquid Separator

B2, B7, B8: Liquid-Liquid Separator

Figure 1. Coffee Extraction Simulation Scheme

2.2.3. Operating Conditions and Sensitivity Analysis

Every simulation was done at atmospheric pressure. The temperature was adjusted to 40, 50, and 60°C to indicate an average operating temperature that is normally used in the extraction system based on ethanol [21], [22], [23]. S/F mass ratio was varied at 1:1, 2.5:1, and 5:1 to investigate how the availability of solvent had an impact on stagewise separation behavior. The results were assessed on a per-stage basis. The sensitivity analysis investigated the effect of operating conditions and uncertainty of thermodynamic parameters on separation performance. There were three variables used; these were temperature, solvent-to-feed ratio, and binary interaction parameters. Systematic variation of temperature and S/F ratio was done over the predetermined ranges. Moreover, parameters of selected NRTL binary interactions were disturbed by -10% and +10% than their initial values. This analysis was meant to test the strength and stability of projected trends and not to determine the optimum operating conditions [24].

2.2.4. Calculation of Oil Recovery and Total Impurity Removal

As Oil recovery at a given stage i was calculated based on the cumulative mass of lipid components recovered in the lipid-rich phase relative to the total lipid mass introduced with the feed:

$$\text{Oil Recovery}_i\ (\%) = \frac{\sum m_{\text{lipid},\,i}^{\text{recovered}}}{\sum m_{\text{lipid}}^{\text{feed}}} \times 100 \qquad (1)$$

where lipid components include TAG, DAG, MAG, and FFA.

Total impurity removal at a given stage i was calculated as the cumulative fraction of impurity components transferred out of the lipid-rich phase:

$$\text{Impurity Removal}_i\ (\%) = \left(1 - \frac{\sum m_{\text{impurity},\,i}^{\text{lipid phase}}}{\sum m_{\text{impurity}}^{\text{feed}}}\right) \times 100 \qquad (2)$$

where impurity components include caffeine, CGA, and cafestol.

All values reported for sensitivity analysis correspond to cumulative performance up to the specified

3. RESULT AND DISCUSSION

3.1. Coffee Oil Specification

In this work, coffee oil refers operationally to the lipid-rich fraction which can be extracted by ethanol-based processing conditions of SCG, and not to one particular chemical species. A set of major lipid classes, such as TAGs, DAGs, MAGs, and FFA, in the simulation represented the lipid fraction. All these components make up the target product of the separation process and thus were lumped and considered as a total oil recovery to make performance judgments. This lumped description is in line with equilibrium-based studies of processes, in which the goal is to determine the behavior of bulk separation and not the detailed behavior of lipid speciation [9].

On the other hand, a few non-lipid compounds that were inherent in SCG were specifically considered as impurities when it comes to the separation of coffee oil. Caffeine, CGA, and cafestol were chosen as typical polar and semi-polar substances since they are reported to co-extract with ethanol and are commonly identified as being bitter, constrained in their regulatory or oleochemical utility, or less suitable to oleochemical uses of coffee oil [8], [19], [23]. The separate performance of these compounds was monitored in the simulation because of the individual behavior of the compounds at the equilibrium, but the performance of the impurities was reported in the cumulative mode to indicate the overall performance of separation. It is pointed out that the fact that caffeine, CGA, and cafestol were classified as impurities is purely application-specific and does not mean that these compounds are not valuable in themselves. Instead, under the context of this research, impurity removal is the process of their separation with the fatty fraction in order to enhance the quality composition of coffee oil. Chemical degradation or conversion of these compounds was not assumed or modeled; these compounds are only separated by means of partitioning between the solid phase and the solvent phase by equilibrium.

Thermodynamically, ethanol has a high degree of polarity and thus it can dissolve lipid and polar constituents of SCG, especially when in multistage contact. Accordingly, there is not sharp selectivity at separation, but there is progressive redistribution of the components at different stages toward equilibrium. This action lies at the basis of the reasoning of leaching stages (Stages 1-2) where non-selective leaching is predominant, and purification stages (Stages 3 5) where a balance between lipid-rich and impurity-rich fractions is more evidently controlled by LLE. Equilibrium analyses of the refining of vegetable oils, bioactive compounds extraction, and multistage liquid-liquid separation systems have also used these similar structures with the polar co-components extracted progressively in the later stages and the recovery of oil decreases because of the redistribution effects of the solvents. The impurity and oil definitions employed in this paper thus offer a solid foundation in interpreting the stage results and in trade-offs between the separation efficiency and lipid retention without extrapolating claims to equilibrium behaviour.

3.2. Influence of Operating Conditions on Impurities Removal

The effect of operating conditions on the removal of impurities has a well-defined stage-dependent character, with such effects getting increasingly weaker as the extraction system moves out of the washing-dominated regime to the separation-dominated regime. It is observed that this tendency shows the shift of the role of solvent availability and equilibrium partitioning as the process moves through consecutive stages.

Table 3. Simulation and Sensitivity Results of Caffeine, CGA, and Cafestol Removal

No of Case	**S/F Ratio**	**Temp (°C)**	**Removal of Total Caffeine, CGA, and Cafestol (w/w)***		
			Original BIP	**BIP -10%**	**BIP + 10%**
Stage 3					
1	1:1	40	97.14%	96.56%	97.63%
2	1:1	50	97.28%	96.60%	97.57%
3	1:1	60	97.37%	96.49%	97.56%

No of Case	S/F Ratio	Temp (°C)	Removal of Total Caffeine, CGA, and Cafestol (w/w)*		
			Original BIP	**BIP -10%**	**BIP + 10%**
4	2.5:1	40	98.86%	97.77%	98.91%
5	2.5:1	50	98.93%	98.04%	98.99%
6	2.5:1	60	99.00%	98.21%	99.10%
7	5:1	40	99.05%	98.55%	99.15%
8	5:1	50	99.06%	98.56%	99.26%
9	5:1	60	99.10%	98.60%	99.30%
Stage 4					
1	1:1	40	99.91%	99.31%	99.92%
2	1:1	50	99.92%	99.22%	99.94%
3	1:1	60	99.94%	99.04%	99.96%
4	2.5:1	40	99.98%	98.88%	99.99%
5	2.5:1	50	99.98%	99.08%	99.99%
6	2.5:1	60	99.98%	99.18%	99.99%
7	5:1	40	99.99%	99.49%	99.99%
8	5:1	50	99.99%	99.49%	99.99%
9	5:1	60	99.99%	99.49%	99.99%
Stage 5					
1	1:1	40	99.99%	98.94%	99.99%
2	1:1	50	99.99%	98.99%	99.99%
3	1:1	60	99.99%	99.02%	99.99%
4	2.5:1	40	99.99%	99.09%	99.99%
5	2.5:1	50	99.99%	99.12%	99.99%
6	2.5:1	60	99.99%	99.19%	99.99%
7	5:1	40	99.99%	99.49%	99.99%
8	5:1	50	99.99%	99.53%	99.99%
9	5:1	60	99.99%	99.54%	99.99%

At Stage 3, the removal of impurities is moderately affected by the S/F ratio. Table. 3 illustrates that an increase of the S/F ratio to 5:1 increases the cumulative removal of caffeine, CGA, and cafestol to about 97 to 99 %(w/w). This reaction is indicative that at the end of the initial washing steps, a portion of polar and semi-polar compounds is still loosely held by the lipid-rich layer or still embedded within the solid matrix [25], [26], [27]. Additional solvent at this stage promotes better phase contact, and additional redistribution of these remaining impurities to the solvent phase [28], [29]. The scale of this increase is however, also not very high, pointing to the fact that much of the cleaning of impurities has already been done upstream.

Conversely, the change in temperature in the studied range of 40- 60 °C has a slight effect on the removal of impurities at Stage 3. The comparatively minor temperature effect means that, at the chosen solvent system, the equilibrium partitioning of the desired impurities is directed by solvent-solute affinity as opposed to temperature-induced modifications in the solubility [14]. This observation can be associated with equilibrium-based extraction systems where the moderate temperature variations do not significantly affect the phase behavior as long as solvent polarity does not change. Stages 4 and 5 the impurity removal sensitivity of the S/F ratio and temperature becomes insignificant. Stage 4 impurity removal is uniformly high in all operating conditions tested (removal is above 99.99%) with Stage 5 appearing to exhibit an apparent asymptotic behavior (removal is around 99.99%).

Table 4. Simulation and Sensitivity Results of Caffeine, CGA, and Cafestol Removal

No of Case	**S/F Ratio**	**Temp (°C)**	**Oil Recovery (w/w)***		
			Original BIP	**BIP -10%**	**BIP + 10%**
1	1:1	40	69.11%	68.22%	69.87%
2	1:1	50	67.35%	66.40%	67.55%
3	1:1	60	66.67%	65.94%	66.74%
4	2.5:1	40	64.23%	63.58%	64.55%
5	2.5:1	50	63.51%	62.94%	63.57%
6	2.5:1	60	62.68%	62.12%	63.31%
7	5:1	40	60.33%	59.61%	60.45%
8	5:1	50	59.45%	58.91%	59.63%
9	5:1	60	58.12%	57.82%	58.23%

***at the fifth stage of coffee oil purification**

The insensitivity of removal efficiencies to operating conditions indicates that the system has an effective equilibrium limit as far as impurity partitioning is concerned. With these conditions, additional rises in the flow of solvents or temperature have little influence on the degree of impurity separation, but on the solvent circulation and redistribution of internal mass [14], [30].

Significantly, this plateau behavior does not mean that the impurity is completely purified, but the fact that the impurity removal is less sensitive to operational intensification in the modeled equilibrium. The same trends have been observed in the case of multistage liquid-liquid extraction and leaching experiments, where the polar compounds that are easy to extract are extracted at an earlier stage, and the latter stages are operated to approach equilibrium limits and not to yield stepwise increases in separation. In this context, Stage 4 can be regarded as the beginning of a separation plateau, beyond which other stages or more extreme operating conditions will give low marginal returns in terms of impurity removal, but which may raise solvent demands as well.

3.3. Trade-Off between Separation Performance and Oil Recovery

The simulation findings show that there is a steady, equilibrium-based trade-off: the increase in impurity removal is at the cost of lower oil recovery in the purification regime studied, as shown on Table 3. and Table 4**.**. In our cases, the S/F ratio has the greatest effect on the recovery of oil. The current oil recovery values at Stage 5 reduce to about 69.1% (w/w) (Case 1: S/F 1:1, 40 °C) and to about 60.3% (Case 7: S/F 5:1, 40 °C) with the initial BIPs set, and more to about 58.1% at Case 9 (S/F 5:1, 60 °C). This is likely an equilibrium behavior since, with a larger solvent inventory, the overall capability of solutes to be partitioned is greater and is likely to redistribute lipids at any given stage back into the solution; when describing fractional recovery at a given stage number, the redistribution will be seen as reduced fractional recovery despite the total mass of lipids remaining constant.

Another consistent factor is temperature: at the studied 40-60 °C range, the recovers of oil decrease over time with temperature, usually by 1-3 points in percentage between S/F cases Table. 4. Within the used activity-coefficient model, the temperature only has a small effect on solvent-solute interactions and relative partitioning of polar versus nonpolar species, with a slight preference of polar co-components to be partitioned to the solvent and, thus, lowering observed lipid fraction at a given stage. The temperature effect being simulated in our simulations is less than S/F but is not negligible in terms of design trade-offs. Compounds of these tendencies were found in Stage number: Stage 3 generally shows a transition of impurity transfer which is highly complete (97% removal) but still responsive to S/F; Stage 4 shows a plateau of purification (>99.9% removal) and Stage 5 yields marginal progressive purification and reduces the reported oil recovery. Thus, to measure separation performance, it is necessary to report both impurity removal and cumulative recovery (dry-basis) and any design decision must be made against clear goals (target impurity level, permissible recovery loss, solvent requirement). The current findings must be interpreted as a balance inclination instead of being dictatorial forecasts of performance in actual equipment**.**

3.4. Robustness of Thermodynamic Parameters Uncertainty Results

In order to investigate model sensitivity to thermodynamic uncertainty, binary interaction parameters (BIP) were perturbed independently by +10% and -10 %. Perturbations introduced did not cause large changes in the key outputs: the change in oil recovery at the BIP of 10% was usually within the range of 0.5-1.0% point at the BIP of Stages 4-5 (e.g., Case 1 oil recovery: 69.11%(w/w) base to 68.22% at the BIP of -10% and 69.87% (w/w) at the BIP of +10%), and the impurity removed at Stages 4-5 was nearly constant These restricted responses show that qualitative determination of a purification plateau and ranking effects of S/F and temperature are strong to moderate BIP uncertainty in the selected property framework. It is important to note that this strength is directional and comparative conclusions and not absolute numerical fealty. The small sensitivity to the BIP in this article is not a confirmation of the BIP values, but of the fact that under the selected component slate and model of the properties, it is the small perturbation of parameters that does not turn around the trends in the stages.

To ensure reproducibility and auditability, the manuscript has a BIP table of the data sources at Supplementary Table 1**.**, and the stream-by-stream mass balances that were used to compute the reported percentages are in the Suppplementary Table 2. The flowsheet is clear with regard to outlining the progression of solids between stages and fresh solvent being added to each stage as per the designated S/F ratios, and no stream of oil-rich liquid is recovered back into previous mixers. As part of this proper stagewise model, Stage 1-2 are washing steps that diminish the initial load of soluble impurity and Stages 3-5 are dominated by equilibrium-controlled separation behaviour. In practice, working at conditions that force the system into the Stage 4 plateau will be an effective way to efficiently eliminate the tracked polar compounds (>99.9%), although at the cost of bigger solvent inventory and reduced per-stage recovery as reported at a fixed stage number. Stage 4 is thus an informative reference condition for robustness testing, but not an unconditional guideline to industrial practice since equipment reality (entrainment, lack of phase disengagement, solvent retention in solids, solvent recovery duty) will not be reflected in equilibrium calculations. No conclusions about the process level consumption of solvents, the energy requirement or equipment size have to be made until it has been complemented by bench scale separation experiments and solvent recovery estimates.

This study performed an equilibrium-based simulation experiment and restricts the conclusions drawn. The model excludes kinetics (intraparticle diffusion, film resistance), equipment hydrodynamics, separator entrainment fractions, and solvent-hold-up in solids; thus reported oil recoveries and impurity removal values are only to be used as thermodynamic upper limits and trend indicators. It is suggested that specific experimental tasks (moisture and lipid content on a dry basis, TAG/FFA characterization, HPLC quantification of caffeine/CGA/cafestol, separator entrainment tests and residual solvent analysis) be performed prior to the use of the model outputs in scale-up or techno-economic optimization. Letters on reporting and interpretation in the revised manuscript are thus carefully conservative and confined to the insights of equilibrium as backed by the full disclosure of a model

4. CONCLUSION

This simulation study, based on the equilibrium, explains the functionality of the stage and the equilibrium trends of multistage coffee-oil separation of spent coffee grounds with ethanol. In the modeled assumptions (ethanol solvent is modeled, at 96 (%(w/w)), dry-basis feed, explicit component slate including TAG/DAG/MAG/FFA and caffeine/CGA/cafestol), the cumulative removal of impurities is approximately 97% at Stage 3 and more than 99.9% at Stage 4, and the reported recovery of oil is lower with an increased S/F ratio, temperature, and higher stage. Qualitative patterns were not significantly changed using BIPs perturbed by more than +10%. Due to the equilibrium range, all the reported values are reported as thermodynamic tendencies and upper-bound indicators. To be used in engineering, we would suggest experimental anchoring (compositional analysis, kinetic extraction data, and separation/entrainment testing) and a process-level solvent recovery analysis before any operations recommendations are made.

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APPENDIX

Supplementary Table 1. BIPS value

Component i	Component j	BIJ	BJI	CIJ	T
WATER-02	ETHAN-01	463.937.495	432.668.536	0.3	40
WATER-02	TRILI-01	174.170.663	943.981.503	0.3	40
WATER-02	TRIPA-01	152.940.706	936.838.691	0.3	40
WATER-02	1:2-D-02	10.774.488	691.875.197	0.3	40
WATER-02	1:2-D-01	938.003.094	658.030.384	0.3	40
WATER-02	MONOLINO	531.099.316	420.752.182	0.3	40
WATER-02	LINOL-01	488.935.024	829.946.362	0.3	40
WATER-02	PALMITIC	419.559.827	738.933.072	0.3	40
ETHAN-01	TRILI-01	330.794.953	224.934.865	0.3	40
ETHAN-01	TRIPA-01	284.722.313	203.087.396	0.3	40
ETHAN-01	1:2-D-02	181.740.488	-134.302.983	0.3	40
ETHAN-01	1:2-D-01	156.609.519	-175.952.763	0.3	40
ETHAN-01	MONOLINO	915.288.279	-368.071.041	0.3	40
ETHAN-01	LINOL-01	918.895.993	-168.400.075	0.3	40
ETHAN-01	PALMITIC	798.633.244	-200.118.181	0.3	40
TRILI-01	TRIPA-01	321.635.293	-263.170.356	0.3	40
TRILI-01	1:2-D-02	-0.020329649	158.646.729	0.3	40
TRILI-01	1:2-D-01	-390.731.469	199.422.501	0.3	40
TRILI-01	MONOLINO	282.843.635	716.799.873	0.3	40
TRILI-01	LINOL-01	-201.097.168	25.310.934	0.3	40
TRILI-01	PALMITIC	-295.067.994	394.091.644	0.3	40
TRIPA-01	1:2-D-02	501.382.634	899.256.166	0.3	40
TRIPA-01	1:2-D-01	262.123.616	150.734.556	0.3	40
TRIPA-01	MONOLINO	316.816.137	600.250.299	0.3	40
TRIPA-01	LINOL-01	163.488.098	-101.682.347	0.3	40
TRIPA-01	PALMITIC	-156.140.469	258.449.363	0.3	40
1:2-D-02	1:2-D-01	233.580.782	-199.749.895	0.3	40
1:2-D-02	MONOLINO	18.122.136	24.596.197	0.3	40
1:2-D-02	LINOL-01	737.190.289	-498.851.785	0.3	40
1:2-D-02	PALMITIC	891.171.498	-566.772.977	0.3	40
1:2-D-01	MONOLINO	215.208.244	180.583.094	0.3	40
1:2-D-01	LINOL-01	68.647.802	-471.867.265	0.3	40
1:2-D-01	PALMITIC	736.163.901	-497.124.442	0.3	40
MONOLINO	LINOL-01	-165.104.439	247.318.313	0.3	40
MONOLINO	PALMITIC	456.318.087	-33.967.177	0.3	40
LINOL-01	PALMITIC	200.971.875	-175.081.519	0.3	40

Supplementary Table 2. Tables of Results

Parameter	Units	SCG	ETHANOL	ETHANOL2	ETHANOL3	ETHANOL4	ETHANOL5
From							
To		MIXER1	MIXER1	MIXER2	MIXER3	MIXER4	MIXER5

Parameter	**Units**	**SCG**	**ETHANOL**	**ETHANOL2**	**ETHANOL3**	**ETHANOL4**	**ETHANOL5**
Stream Class		MIXNC	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Total Stream							
Temperature	C	30.00	30.00	30.00	30.00	30.00	30.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01	1.01
Mass Liquid Fraction		0.22	1.00	1.00	1.00	1.00	1.00
Mass Solid Fraction		0.78	0.00	0.00	0.00	0.00	0.00
Mass Flows	kg/hr	1.00	2.50	0.82	0.72	2.50	2.50
Mass Fractions							
WATER-02		0.00	0.04	0.04	0.04	0.04	0.04
ETHAN-01		0.00	0.96	0.96	0.96	0.96	0.96
TRILI-01		0.09	0.00	0.00	0.00	0.00	0.00
TRIPA-01		0.08	0.00	0.00	0.00	0.00	0.00
1:2-D-02		0.01	0.00	0.00	0.00	0.00	0.00
1:2-D-01		0.01	0.00	0.00	0.00	0.00	0.00
MONOLINO		0.01	0.00	0.00	0.00	0.00	0.00
MONOPALM		0.01	0.00	0.00	0.00	0.00	0.00
LINOL-01		0.01	0.00	0.00	0.00	0.00	0.00
PALMITIC		0.01	0.00	0.00	0.00	0.00	0.00
CAFFEINE		0.00	0.00	0.00	0.00	0.00	0.00
CHLO-ACD		0.00	0.00	0.00	0.00	0.00	0.00
CAFESTOL		0.00	0.00	0.00	0.00	0.00	0.00
SCG-MTRX		0.78	0.00	0.00	0.00	0.00	0.00
Parameter	Units	1	2	3	4	5	
From		MIXER1	MIXER2	MIXER3	MIXER4	MIXER5	
To		B1	B2	B3	B6	B7	
Stream Class		MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	
Total Stream							
Temperature	C	30.01	37.49	38.01	30.41	30.41	
Pressure	bar	1.01	1.01	1.01	1.01	1.01	
Mass Liquid Fraction		0.78	0.99	1.00	1.00	1.00	
Mass Solid Fraction		0.22	0.01	0.00	0.00	0.00	
Mass Flows	kg/hr	3.50	3.30	3.66	2.66	2.66	
Mass Fractions							
WATER-02		0.03	0.04	0.04	0.04	0.04	
ETHAN-01		0.69	0.89	0.91	0.91	0.91	
TRILI-01		0.03	0.03	0.02	0.03	0.03	
TRIPA-01		0.02	0.02	0.02	0.03	0.02	
1:2-D-02		0.00	0.00	0.00	0.00	0.00	
1:2-D-01		0.00	0.00	0.00	0.00	0.00	
MONOLINO		0.00	0.00	0.00	0.00	0.00	
MONOPALM		0.00	0.00	0.00	0.00	0.00	
LINOL-01		0.00	0.00	0.00	0.00	0.00	
PALMITIC		0.00	0.00	0.00	0.00	0.00	
CAFFEINE		0.00	0.00	0.00	0.00	0.00	
CHLO-ACD		0.00	0.00	0.00	0.00	0.00	

Parameter	**Units**	**SCG**	**ETHANOL**	**ETHANOL2**	**ETHANOL3**	**ETHANOL4**	**ETHANOL5**
CAFESTOL		0.00	0.00	0.00	0.00	0.00	
SCG-MTRX		0.22	0.01	0.00	0.00	0.00	
Parameter	Units	OIL1	OIL2	OIL3	OIL4	OIL5	
From		B1	B2	B3	B6	B7	
To		MIXER2	MIXER3	MIXER4	MIXER5		
Stream Class		MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	
Total Stream							
Temperature	C	40.00	40.00	40.00	40.00	40.00	
Pressure	bar	1.01	1.01	1.01	1.01	1.01	
Mass Liquid Fraction		0.98	1.00	1.00	1.00	1.00	
Mass Solid Fraction		0.02	0.00	0.00	0.00	0.00	
Mass Flows	kg/hr	2.49	2.94	0.16	0.16	0.15	
Mass Fractions							
WATER-02		0.04	0.04	0.00	0.00	0.00	
ETHAN-01		0.87	0.90	0.08	0.07	0.07	
TRILI-01		0.03	0.03	0.48	0.49	0.49	
TRIPA-01		0.03	0.02	0.42	0.42	0.42	
1:2-D-02		0.00	0.00	0.01	0.01	0.00	
1:2-D-01		0.00	0.00	0.01	0.00	0.00	
MONOLINO		0.00	0.00	0.00	0.00	0.00	
MONOPALM		0.00	0.00	0.00	0.00	0.00	
LINOL-01		0.00	0.00	0.00	0.00	0.00	
PALMITIC		0.00	0.00	0.00	0.00	0.00	
CAFFEINE		0.00	0.00	0.00	0.00	0.00	
CHLO-ACD		0.00	0.00	0.00	0.00	0.00	
CAFESTOL		0.00	0.00	0.00	0.00	0.00	
SCG-MTRX		0.02	0.00	0.00	0.00	0.00	
Parameter	Units	RESIDU	RESIDU2	RESIDU3	RESIDU4	RESIDU5	
From		B1	B2	B3	B6	B7	
To							
Stream Class		MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	
Total Stream							
Temperature	C	40.00	40.00	40.00	40.00	40.00	
Pressure	bar	1.01	1.01	1.01	1.01	1.01	
Mass Liquid Fraction		0.27	0.89	1.00	1.00	1.00	
Mass Solid Fraction		0.73	0.11	0.00	0.00	0.00	
Mass Flows	kg/hr	1.01	0.37	3.50	2.50	2.50	
Mass Fractions							
WATER-02		0.01	0.03	0.04	0.04	0.04	
ETHAN-01		0.24	0.81	0.95	0.96	0.96	
TRILI-01		0.01	0.02	0.00	0.00	0.00	
TRIPA-01		0.01	0.02	0.00	0.00	0.00	
1:2-D-02		0.00	0.00	0.00	0.00	0.00	
1:2-D-01		0.00	0.00	0.00	0.00	0.00	
MONOLINO		0.00	0.00	0.00	0.00	0.00	

Parameter	Units	SCG	ETHANOL	ETHANOL2	ETHANOL3	ETHANOL4	ETHANOL5
MONOPALM		0.00	0.00	0.00	0.00	0.00	
LINOL-01		0.00	0.00	0.00	0.00	0.00	
PALMITIC		0.00	0.00	0.00	0.00	0.00	
CAFFEINE		0.00	0.00	0.00	0.00	0.00	
CHLO-ACD		0.00	0.00	0.00	0.00	0.00	
CAFESTOL		0.00	0.00	0.00	0.00	0.00	
SCG-MTRX		0.73	0.11	0.00	0.00	0.00	