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A Generalized Optimization Approach for the Characterization of Non-Conventional Streams

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ABSTRACT

This study provides standardized models for the chemical characterization of complex streams, ensuring the necessary adaptations while considering the differences in biomass types and forms. Several datasets are compiled and examined to establish a valid representation of the mixture, according to industry accepted standards and laboratory protocols. For reliable property estimation, correlations of key biomass properties are obtained from both computational models and experimental measurements. Existing data are used to create datasets for the biomass and the biocrude streams. This model builds upon existing knowledge and data technologies with emphasis on hydrothermal liquefaction (HTL). The proposed approach shows potential as a starting point for the design and modelling of more biorefinery-associated technologies. Sludge and pine wood are used as case studies for biomass feedstocks. Two biocrude samples are employed for biocrude characterization. The performance of the developed optimization model is compared favorably with results obtained using previous works. To ensure a variety of possible and valid solutions, integer cuts are implemented producing solution pools for the analysed streams.

Keywords: Optimization, MINLP, Biomass, Biorefineries, Biocrude, Integer cuts

INTRODUCTION

Global emissions have increased rapidly over the last half-century, driving climate change [1]. Fossil fuels are by far the largest contributor, accounting for over 75% of global greenhouse gas emissions and nearly 90% of all CO_2 emissions [2]. Bioenergy offers a sustainable alternative, potentially supplying a quarter to a third of global primary energy by 2050 and replacing fossil fuels across energy markets [3]. Second-generation biorefinery processes convert a range of organic feedstocks into biocrude, which can be upgraded into liquid hydrocarbon fuels [4].

Among these, hydrothermal liquefaction (HTL) is a promising technology for converting biomass into biocrude and valuable chemicals under high temperature and pressure conditions [5]. The process offers advantages such as wet biomass processing and reduced tar formation [6] and is easily adaptable to various types of biomass feedstocks [7]. The reaction mechanisms involve depolymerization of biomass components, with proteins, lipids, and carbohydrates following distinct pathways [8]. Some HTL fuels can reduce Global Warming Potential by approximately 70% compared to conventional jet fuel [9].

Mechanistic kinetic models have been developed for HTL, to predict product yields and composition for different feedstocks [10]. Characterization of the biomass and biocrude streams is crucial for modeling the complexity of HTL reaction mechanisms and upgrading the process [11]. Various analytical methods can be employed, including conventional analytical methods like GC, FTIR, and NMR, or advanced 2D- GC, LC, NMR and HRMS techniques [12]. Conventional methods face limitations in comprehensively characterizing the complex composition of these streams, requiring advanced techniques to produce comprehensive results [13].

Stream characterization can also be done using computational techniques (in the form of optimization or Machine Learning models) using experimental datasets containing information relevant to each studied system [14-16]. A common limitation across all methods mentioned is the inadequacy of available data, tools and flow sheeting techniques for accurately representing different biomass types.

Park et al. (2023) employed HPLC derived data to develop predictive equations correlating biochemical content with elemental composition in biomass characterization [17]. Ahmed et al. (2019) relied on machine learning techniques to estimate moisture content and compositional analysis based on data derived from NIR spectroscopy [18]. Taghipour et al. (2021) characterized biocrude streams through multi-objective optimization with the NSGA-II algorithm, by integrating distillation data [19]. Aslanoglou et al. (2024) proposed a model that utilizes both stochastic and deterministic algorithms to simulate the input and output streams associated with hydrothermal liquefaction (HTL) of sewage sludge [20].

This work builds on existing models and data to develop a robust generalized optimization model, to capture the composition diversity and characterize biomass and biofuel streams. The following sections present the proposed methodology and the material datasets utilized here, compare the model performance to previous works, and illustrate the use of integer cuts to deliver portfolios of solutions.

METHODOLOGY

This section describes the mathematical model developed here for the characterization and analysis of biomass and biocrude streams and its implementation.

The objective function F is formulated as follows:

$$min\{F\} = \sum_{m=1}^{M}\left(1 - f_m/\hat{f}_m\right)^2 + \sum_{k=1}^{K}\left(1 - f_k/\hat{f}_k\right)^2 \quad (1)$$

where $\hat{f}$ and f denote experimental and first principle based data for each property $k \in \{1, \ldots, K\}$ and $m \in \{1, \ldots, M\}$, respectively.

The following sets of properties are considered:

- Elemental composition of m={Carbon, Hydrogen, Oxygen, Nitrogen, Sulfur,..} where $Nm_{m,j}$ denotes the number of elements in every compound and Ar_m the element atomic number.

$$f_m = \frac{\sum_j x_j \cdot Nm_{m,j} \cdot Ar_m}{\sum_{m=1}^{M} \sum_j x_j \cdot Nm_{m,j} \cdot Ar_m} \quad (2)$$

- Biochemical composition k={Protein, Carbohydrate, Lignin, Lipid, etc.} where $B_{k,j}$ denotes the biochemical identification in every compound.

$$f_k = \sum_j x_j \cdot B_{k,j} \quad (3)$$

where x_j denotes the composition of compound j.

- The model can also incorporate constraints on the stream property values, to ensure that they match experimental characterization data. These properties may include Higher Heating Values (HHV), densities and Boiling Point Temperature (TBP) profiles (only for biocrude mixtures).

Feasibility constraints are also applied:

$$\begin{pmatrix} I & -L_x I \\ -I & U_x I \end{pmatrix} \begin{pmatrix} x_j \\ y_j \end{pmatrix} \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (4)$$

where y_j is a binary variable indicating the presence of a compound in the mixture; L_j and U_j are the lower and upper bound of the continuous variable x_j.

$$\sum_j x_j = a, \quad a \leq 1 \quad (5)$$

$$\sum_j y_j \leq N \quad (6)$$

where a is the total dry and ash-free composition.

The above are implemented in GAMS as a mixed-integer nonlinear programming (MINLP) problem solved using the BARON solver. The model inputs are the feedstock and biocrude properties. The model outputs are estimates of the unknown feedstock composition.

The model is solved iteratively to produce multiple solutions through integer cuts, resulting in alternate populations that match optimization requirements. We also apply integer cuts to generate a set of alternative stream compositions and investigate governing stream characteristics [21]. Algorithm 1 shows a pseudocode of the algorithm to solve the MINLP problem of Equations 1-6, including the integer cuts.

Algorithm 1: Implementation of the optimization model

```
Data input
    Read compound dataset, D=[C×K]
    Read stream property data, PD=[K×1]
MINLP model definitions
    Property models, PM=[K×1]
    Objective function F = f(X), X=[C×1]
    Property Constraints G = g(X,Y), Y=[C×1]
    Feasibility constraints H = h(X,Y)
Integer cuts definitions
    Number of runs, N
    Min differences per solution, M
    Initial solution table, T=[N×C]
Loop {n=1 to N}
    Solve MINLP model so that
        |Yn-Yi|≥M, for all i∈{1,…,n-1}
    Output the estimated composition Xn=[C×1]
Next n
```

DATASETS

Two distinct datasets are used for stream characterization for biocrude (Table 1) and biomass (Table 2). Data on selected chemicals are collected from published works providing experimental (e.g. HPLC) and simulation data (e.g. Optimization) for biomass [20, 22-30] and biocrude [19, 20, 31, 32] characterization.

Table 1: Biocrude dataset description (144 compounds)

Saturated hydrocarbons; aromatic compounds etc.
Molecular weight ranges: 60-410 g/mol
TBP ranges: 50-550^{o}C
Properties (molecular weight, TBP, SMILES etc).

Table 2: Biomass dataset description (111 compounds)

18% amino acids
23% carbohydrates
31% lipids
28% lignin compounds
Molecular weight ranges: 70-600 g/mol
Density ranges: 0.8-1.7 g/cm3
Properties (chemical formula, density, SMILES etc).

CASE STUDIES

Biomass characterization

We showcase the versatility and wide applicability of the proposed MINLP model by examining three sludge and pine wood feedstocks, which exhibit significant differences in protein and lignin content. In all three cases, we consider the biomass dataset of Table 2. When the compositions don't add up to 100% the model is adjusted to consider normalized values.

Case F1: Table 3 shows the obtained deviations between experimental and calculated values for the sewage sludge. The MINLP results are tested against those of Aslanoglou et al. (2024) who compared two evolutionary (firefly algorithm (FA) and particle swarm optimization (PSO)) and two deterministic algorithms (sequential quadratic programming (SQP) and least squares optimization (LS)). SQP had the best performance using a dataset tailored to sludge streams [20]. The current model outperforms significantly their best model (SQP) in fitting to the experimental values. We finally observe that the overall objective function value is reduced here by 93%.

Table 3: Comparison of biomass results in case F1

	Exp. Data	SQP		MINLP	
Carbon	54.20	52.36	3.40%	54.47	0.49%
Hydrogen	7.30	7.43	1.77%	7.30	0.00%
Oxygen	34.20	36.85	7.73%	34.63	1.26%
Nitrogen	3.60	3.25	9.78%	3.60	0.00%
proteins	15.77	17.42	10.44%	15.39	2.42%
H/C	40.58	42.66	5.13%	41.47	2.20%
lipids	13.06	13.45	3.00%	12.67	2.95%
Lignin	25.10	26.47	5.46%	24.97	0.51%
HHV	24.51	23.71	3.24%	24.62	0.47%
SSRD			3.55E-02		2.17E-03

Case F2: This case considers a pine wood sample from Obeid et al. (2021) (Type: Sawdust) [33]. Table 4 reports an excellent fit to the experimental values. In this case we did not have information on the mixture HHV.

Case F3: Table 5 reports the MINP model results for a sludge stream from Snowden-Swan et al. (2022) (Type: WW09 50/50 CCSD, DAF) [34]. In this case we also demonstrate the use of integer cuts. Table 5 reports the overall results statistics for 50 solutions of the MINLP model. Here we obtain a distribution of values for the elementary and the biochemical compositions, so we report the average and the standard deviations of SSRD.

Table 4: Results for the pine wood stream F2

	Exp. Data	MINLP	
Carbon	44.68	43.69	2.21%
Hydrogen	6.15	6.13	0.30%
Oxygen	51.43	50.12	2.55%
Nitrogen	0.06	0.06	0.00%
proteins	0.50	0.50	0.10%
H/C	66.90	76.38	14.17%
lipids	2.80	2.82	0.59%
Lignin	19.50	20.31	4.13%
SSRD			2.30E-02

Table 5: Results for the sludge stream F3

	Exp. Data	MINLP (average & st.dev.)	
Carbon	51.10	51.50	0.009
Hydrogen	7.40	7.41	0.004
Oxygen	35.60	35.79	0.009
Nitrogen	5.30	5.31	0.003
proteins	45.40	45.42	0.031
H/C	46.10	46.08	0.030
lipids	8.00	8.00	0.005
Lignin	0.50	0.50	0.000
SSRD		7.93E-05	5.41E-06

Figure 1 shows the boxplots of the compound concentrations (wt/wt) in the obtained results, which also show the frequency of compound appearance. Note that, we hide the compounds which are not present in any of the 50 solutions. It is observed that, among the lipids, Lignoceric acid and Docosahexanoic acid are the compounds with the highest concentrations (average 3% and 2% respectively). Among the carbohydrates, Cellobiose and Sucrose were found with the highest concentration with an average of 11% and 7% respectively. The most common amino acids found were Phenylalanine and Tyrosine with average values of 12% and 10%.

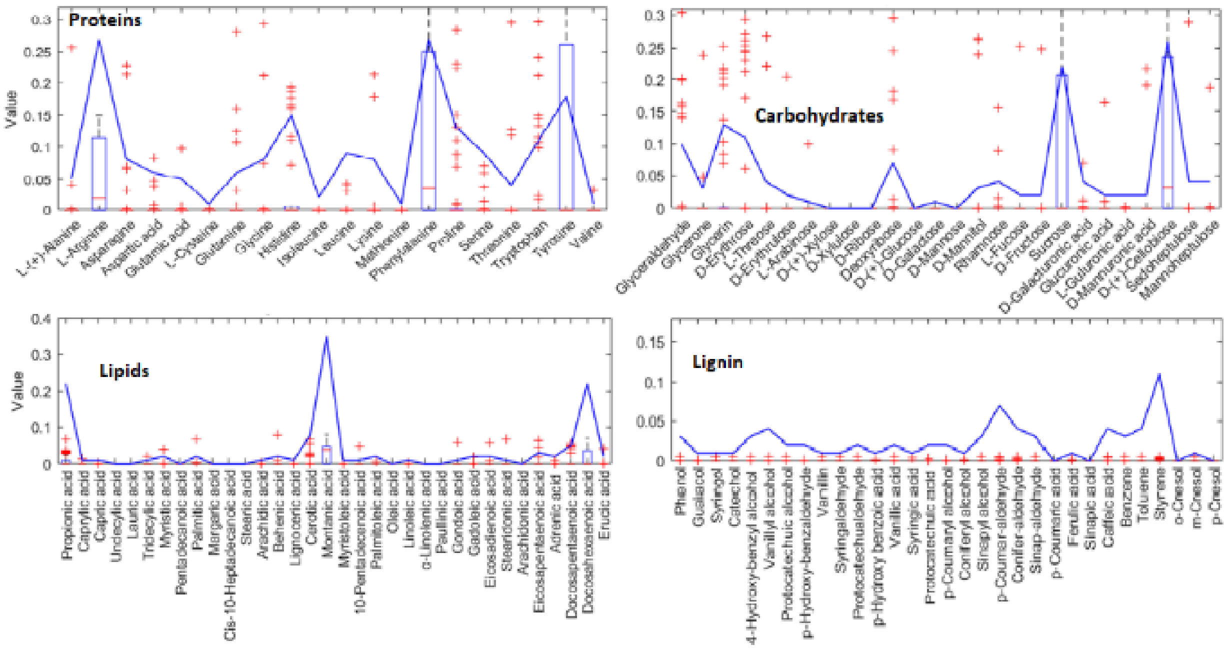
Biocrude characterization

Cases B1 & B2: This case considers Aslanoglou et al. [20]. Table 6 reports an excellent fit to the experimental values. We observe 96% and 78% reductions of the objective function value compared to previous works on biocrude and upgraded biocrude, respectively.

DISCUSSION

The performance of the model developed here is demonstrated on 3 different feedstocks, showing significantly lower deviations compared to previous works. Though we have a limited pool of results, the model seems to perform slightly better in sludge samples, compared to pine wood. This could be attributed to the higher lignin content in wood and woody biomass mixtures, which is more

Figure 1: Boxplots of compound concentrations (wt/wt).



challenging to model effectively, especially considering the structural randomness of its branched topology, as well as its diverse chemical behaviour [35].

Table 6: Results for the biocrude streams B1 and B2

		Exp. Data	LS		MINLP	
Biocrude	Carbon	74.67	75.38	0.95%	75.68	1.35%
	Hydrogen	10.30	10.70	3.88%	10.28	0.16%
	Oxygen	11.30	11.30	0.00%	11.28	0.17%
	Nitrogen	2.76	2.99	8.44%	2.76	0.04%
	HHV	33.20	33.49	0.87%	33.63	1.30%
	SSRD			8.80E-03		3.57E-04

		Exp. Data	SQP		MINLP	
Upgraded biocrude	Carbon	86.20	85.41	0.92%	85.22	1.13%
	Hydrogen	13.00	13.56	4.31%	13.96	7.41%
	Oxygen	0.70	0.78	11.00%	0.71	1.64%
	Nitrogen	0.10	0.11	11.00%	0.10	0.40%
	HHV	38.06	37.71	0.92%	37.62	1.16%
	SSRD			2.62E-02		6.04E-03

Integer cuts would provide (i) multiple feasible solution points that could establish key chemical components (ii) broader potential for data manipulation and machine learning implementation (iii) increased flexibility in choosing appropriate biomass profiles based on fuel or process requirements. Producing alternate populations of components, rather than single options, enhances the comprehensive understanding of complex streams, allowing complementary information to form holistic knowledge in the optimization and design of sophisticated chemical dynamics. The MINLP model was also tested in two biocrude samples.

The proposed MINLP model efficiently produces the chemical profiles of different biomass types and product streams, allowing for a more generalized approach in biorefinery understanding. This model can be adapted for various non-conventional mixtures by incorporating diverse substrate properties, allowing for a broader physiochemical representation. Thus, allowing its applicability across a wide range of biorefinery technologies.

CONCLUSIONS AND FUTURE WORK

Efficient modelling of non-conventional streams requires a comprehensive analysis of first principle models along with experimental data, in accordance with industry accepted standards and laboratory protocols. The purpose is to match the experimental properties of the input or output stream to a mixture of appropriate chemical compounds and functional groups.

This work proposes a new MINLP formulation for the characterization and analysis of biomass and biocrude steams in HTL. Our analysis capitalizes on a combination of peer-reviewed references, experimental, simulation data and relevant databases to acquire specification parameters such as experimental measurements (e.g. moisture content), stoichiometric composition showcasing elemental ratios within samples, as well as thermodynamic properties associated with bioconversion technologies. Classifying biomass feedstocks, requires the chemical compounds to be divided into four biochemical categories, such as proteins, sugars, lipids and lignin.

Accurate representation of complex mixtures in all stages of the biomass conversion process would facilitate decision-making while also providing insight in reaction pathways, which signifies an industrial milestone for biorefinery commercialization.

Decomposition of feedstock streams into chemical compounds allows the modularization of the chemical profile which can be used to redefine information into digital forms, while also creating collective databases of different material mixtures. In essence, digital passports to simplify biomass and biocrude classification.

Ongoing work also considers the incorporation of additional properties to improve accuracy, and also include TBP data to enable fitting to the experimental TBP curve for biocrude streams.

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