Lumped product kinetic model studying interactions during hydrothermal liquefaction of polypropylene – polycarbonate – cellulose mixtures

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## Introduction:

Hydrothermal liquefaction (HTL) valorizes municipal waste such as plastics and biomass to energy rich oil which can act as a crude oil replacement1–3. HTL breaks down carbonaceous feedstocks in sub-critical and super-critical water into four phases of products – oil, aqueous, solid, and gas1. The water serves as both a reactant and solvent4.

When single plastics undergo HTL, they produce oil in supercritical conditions (T> 374 °C, P > 22.12 MPa)5. Whereas HTL of biomass gives higher oil yields under sub- and near-critical conditions1. Upon adding biomass to plastics, the oil yield increases from HTL of mixture when compared to weight averaged oil yield from single component HTL experiments5. For example, HTL of equi-mass PP – cellulose mixture gives higher oil yields than average of oil yields from HTL of PP alone and HTL of cellulose alone at same process conditions5. We call these synergistic increases in oil yield. This leads to higher energy recoveries in sub- and near- critical conditions5. There are also interactions among plastics, and among different biomass components that influence the product distribution5. Hence, understanding and modeling these interactions is pivotal to co-processing mixed (plastic – biomass) waste streams using HTL.

In HTL literature, component additivity models predict product distributions by including these interactions among different components6–9. Early models in this field studied the interactions among different components of biomass – carbohydrates, lignins, starch, protein and lipids7–9. Seshasayee et al.6 recently extended the model study to include interactions between plastic and biomass and interactions among different plastics during HTL. The author identified interactions between lignocelluloses and all plastics tested (PP, PC, PET, PS) during HTL that led to synergistic increases in oil yield. The model included interactions among different components at sub-, near-, and super-critical temperatures at a single HTL process time (30 mins). The model helps understand nature of interactions at different temperature regimes (sub-, near- and supercritical). However, it gives limited information on time effects and propagation of reaction products across the different phases – solid, aqueous, gas.

Kinetic models can serve as an ideal tool to address both these limitations. However, previous kinetic models in HTL are solely developed for biomass and more particularly microalgae10–13. These models are exclusively lumped product kinetic models. This is because HTL of biomass or plastic feedstocks lead to a large number of products. It is hence a difficult task to quantify all different products formed across four different phases.

Most kinetic models developed for HTL do not include interactions among different components as well 10–13. They either consider the feedstock as a monolith or have each of biomass components react independently of each other. Hietala et. al.14, the only exception, included carbohydrate – protein interactions in their model. The author considered carbohydrates, proteins breaking down to saccharides and amino acids and further reacting with each other to form oil. The interactions was modelled as a second order pathway with first order in each saccharide and amino acid. This assumption was made for the simplicity of the model.

Herein in this manuscript, we study the interactional effects in cellulose, polypropylene (PP), and polycarbonate (PC) mixtures. Cellulose, PP, PC are model lignocellulose, polyolefin, and condensation polymer, respectively. We performed HTL experiments on each component alone (i.e., cellulose alone), each equi-mass binary combination (i.e., PP – cellulose (1:1 mixture)) and one equi-mass tertiary combination (PP – PC – cellulose (1:1:1 mixture)) at six different batch holding times (1 – 60 min). We also vary the relative amount of each component in binary mixtures to analyze the ratio effects for each of the interactions through additional experimentation at a fixed batch holding time of 30 mins. All experiments are performed at 350 °C.

A lumped product kinetic model is developed using the unary, binary and ratio experimental results. The kinetic model informs the influence of all three interactions (PP – PC, PP – Cellulose, PC – cellulose) during HTL on all four phases of products. It also estimates the order of reaction for bio-oil pathways. The predictive ability of the model across all phases of products is tested on the tertiary combination experiments. This lumped product kinetic model is the first to model HTL of plastics. This manuscript both studies the nature of interactional effects between plastic and biomass, among different plastics, and models them as well. This also serves as the first kinetic model in HTL to fit order of reaction.

## Methods:

### **Materials:**

Cellulose (microcrystalline, Alfa Aeser), polypropylene and polycarbonate from Sigma Aldrich, were used as received. Reagent grade dichloromethane were procured from VWR International, while deionized water was produced in-house. We constructed 10 mL (internal volume) 316 stainless steel mini-batch reactors from ¾ in. Swagelok parts (a port connector and two caps).

### **Reaction process:**

We load 0.3692 g of feedstock into the mini-batch reactors. In mixture experiments, equal masses of each component are added to attain total feedstock mass loading of 0.3692 g. Water is added to achieve saturation pressure at 350 °C. The reactions are carried out in an isothermal Techne-fluidized sand bath for 1 – 60 mins. Triplicate runs at each condition allows for calculation of the mean value and standard deviation. The temperature profile of the reactor during the heat up process is measured using a dummy reactor loaded with water and equipped with an Omega 1/8 in. Ktype thermocouple.

### **Product work up:**

The contents of the reactor are extracted using 10 mL of dichloromethane (DCM) and 10 mL of deionized water. The DCM soluble phase is termed as the oil phase. Solid products are removed in a 1 µm glass fiber syringe filter from Tisch Scientific (North Bend, OH). The DCM-water mixture is then centrifuged for 8 mins at 3000 RPM. The oil, aqueous and solid phase is recovered and then dried, and the yield is calculated gravimetrically (See Eqn. 1). The gas yields are calculated by difference (100 – oil yield(%) – solid yield(%) – aqueous yield(%)).

[1]

### **Oil phase analysis:**

Compounds in the oil phase are analyzed using Shimadzu GCMS-QP2010 with helium as the carrier gas (flow velocity = 26.5 cm/s). The oven temperature is initially 40 °C for 6 min, followed by a heating ramp of 6 °C/min to 310 °C. The oven is then held at 310 °C for 2 mins. A split injection mode is used for a 5 µL sample injection with a split ratio of 5. The samples are analyzed by the MS detector in full scan mode.

**Kinetic Model Development:**

<Need for ratio effects for improved fit>

## Results and discussion:

**Comparison of oil yield from HTL mixture experiments with single component HTL experiments:**

Fig. 1 indicates process time dependence of oil yields from HTL of PP, PC, cellulose binary and tertiary mixtures. The oil yields from PP alone, PC alone and cellulose alone are given in Fig. S1. The calculated oil yields are mass-averaged oil yields from these single component experiments (see eqn. 2). We conduct t-tests with null hypothesis that difference between experimental and calculated values are zero to check for presence of interaction effects. A (\*\*) mark for an experiment in Fig 1 indicates statistically significant (with p < 0.05) interactions that change oil yields during HTL. An interaction is termed synergistic if it causes an increase in oil yield and termed antagonistic if it causes a decrease in oil yield.



a) PP + Cellulose

b) PC + Cellulose

c) PC + PP

d) PP + PC + Cellulose

Fig. 1: Experimental and calculated oil yields from HTL of a) PP + cellulose, b) PC + cellulose, c) PC + PP and d) PP + PC + Cellulose

[2]

<Temperature profile>

The experiments with process times ranging from 1 – 5 mins are termed as fast HTL experiments while the longer time scales are termed as isothermal HTL. In fast HTL experiments, the reactors do not reach the set point temperature and the temperature keeps increasing throughout the reaction time. We observe characteristic difference in interaction effects between fast and isothermal HTL. For HTL of PP + PC, the interactions are synergistic in fast HTL conditions and then turn antagonistic in isothermal HTL conditions. This might be due to the low depolymerization temperature for PC. HTL of PC alone gives high oil yields (of the order of 30 %) even at 250 °C, 30 mins2. The oil yield from HTL of PC alone further increases to 60 % at 350 °C, 30 mins. Hence, as temperature increases to 350 °C, PC is depolymerizing. Thus, interactions with PP are likely furthering this depolymerization. However, when the temperature increases beyond 350 °C, HTL of PC alone gives oil yields between 50 and 60 %. Thus, no further depolymerization is happening. This might be the reason why PP could be further degrading products formed in oil phase from PP. Note that PP produces very low oil yields at 350 °C. Thus, the oil yield increases and decreases are likely from PC.

Hydrogen abstraction by PC degrades substituted phenolics to phenols15,16. This would incur a loss of oil yield as mass of oil products decrease. This is observed both in the presence of acid catalysts15 and H rich plastics16. PS, PP increased total amount of phenol formed from pyrolysis of PC – PP/PS mixtures16. Note that PP has a H wt. % of 14.2 while PC has a H wt.% of 5.5. Hence, we hypothesize that there is likelihood of transference of H from PP to PC causing a decrease in oil yield. We test this hypothesis by performing HTL of 1:3 tetralin – PC mixture at 350 °C, 30 mins. Tetralin acts as a hydrogen donating agent in this experiment. The experimental oil yield decreases to 42.6 ± 1.93 % which is significantly less than the calculated oil yield for the tetralin – PC mixture (53.84 ± 0.85 %). This observation supports the previous hypothesis regarding the nature of PP – PC interactions during isothermal HTL regime.

However, at shorter times, the same H donation likely causes depolymerization of PC to occur. Previous literature indicates that addition of acid catalysts expedite depolymerization of PC15. Hence, similar to prior corollary for increased formation of phenols, addition of H-rich plastic may increase depolymerization of PC and hence oil yield from PC. To test the hypothesis, we performed short time HTL experiments for PC and tetralin. <perform PC – tetralin short time experiment>

PC + Cellulose mixtures follows a similar trend under fast HTL conditions. Synergistic interactions among cellulose and PC increase oil yield. However, under isothermal conditions, the observations are different. The interactions are antagonistic at 10 mins, non-significant at 30 mins and synergistic at 60 mins. These variations might be due to competing reactions for PC and cellulose that increase and decrease the oil yields. Oil products from PC decompose in this regime due to interactions, which reduces the oil yield. Plastic – biomass interactions also lead to increases in oil yield from biomass. Hence, at longer times, the increase in oil yield from cellulose offshoots the decrease in oil yield from PC. Co-pyrolysis of PC and lignin indicates faster depolymerization of both PC and lignin and higher oil yields from the mixture17,18. Thus, there are prior evidences of PC – biomass interactions accelerating depolymerization of PC. We delve further into this hypothesis during the quantitative GCMS analysis of oil phase section.

For HTL of PP + cellulose mixtures, interactions are synergistic for both fast and isothermal HTL. PP produces low oil yields at 350 C° at all times. The oil yield from HTL of PP alone further increases with temperature until 425 C°. It is still in the depolymerizing at 350 C°. Addition of cellulose is likely further accelerating this process. Hence, in both fast and isothermal HTL, the oil yield increases. Previous literature on pyrolysis of PS – cellulose mixtures indicate increased decomposition of both PS-derived and cellulose-derived products as a result of interactions between the plastic and cellulose19. A similar observation was made also made for PP – PS – Cellulose mixture19. Hence, there are similar observations made in pyrolysis as well. Note that there could also be increases in oil yield from cellulose due to its interaction with PP. We further probe into source of oil yield increases during the discussion of kinetic model and quantitative GCMS analysis.

When, PP, PC, and cellulose are mixed, the interactions are antagonistic at all process times. The decomposition of oil products from PC is promoted by presence of both PP and cellulose. Hence, addition of both these would promote antagonistic interactions – causing decrease in oil yields. Note that ternary interactions among components is also possible. Seshasayee et al. <cite data mining> observed lipid-lignin-protein interactions that increased formation of fatty amines. We hence utilize the kinetic model to predict yields across all phases to also test for presence of any ternary interactions.

**Effect of relative ratio of components on oil yield from HTL:**

Using unary and binary mixture experiments, we fit the kinetic model assuming all reactions are first order. We further modify reaction pathway xx <add number> assuming variable reaction orders on both reactants. Fig. x indicates the <write about fit>

<Order of reaction> <Ratio effects discussion>

**Fit of Kinetic Model for HTL of PP – PC – cellulose mixture:**

Fig. 2 gives the experimental and fitted product yield distribution from kinetic model for HTL of cellulose, PP and PC alone at 350 °C. The experimental and fitted values for each of the cases fit with R2 > 0.8. The average absolute residual between experimental and fitted values for all product distribution are 6.20, 3.90, 1.45 for cellulose, PP, and PC alone. Previous kinetic models for microalgae achieved a R2 fit of 0.4510. Hence, these models achieve greater accuracy on training dataset.

We observe for HTL of cellulose alone and PC alone, there is a clear interplay among all four phases of products. However, for PP alone, the aqueous yields are consistently less than 1 wt.% for all times. Hence, the interplay between phases during HTL is chiefly between oil, solid and gas phases. Note that we are fitting both fast and isothermal HTL using the same kinetic pathway. Using different kinetic constants for the two kinetic regimes might be a potential method to improve model fits at the cost of reducing the degree of freedom. <Test?>

Additional reaction pathways superimpose the unary component (PP, PC, cellulose) alone reaction pathways to include the interactional effects. Note that for the unary component reaction pathways, the kinetic constant values as identified in Fig. a- c are maintained. Fig. S2 gives the model predictions for the binary mixture experiments using reaction pathways from unary component experiments alone <add?>. We see that post addition of these additional pathways; the model fit improves <add couple lines on metrics>. The model fits for HTL of PP + cellulose, PC + cellulose, PP + PC have average absolute residuals of 6.03, 10.48, 6.54, respectively. The R2 values between fit and experimental values are greater than 0.8 for all three binary mixtures.

For PC + cellulose, the model fits well for fast HTL with average absolute residual of 6.91, respectively. However, at longer times, the average absolute errors are larger (15.24). This is likely because the nature of interaction on oil yields changes from being synergistic in fast HTL to antagonistic in isothermal HTL and then synergistic at 60 mins. Such an oscillation of interaction behavior is difficult to capture. To improve this, we utilized different kinetic constant values for fast and isothermal HTL. <add the improved case>.



a) Cellulose

b) PP

c) PC

Fig. 2: Experimental and fitted yields (from kinetic model) of product phases from HTL of a) cellulose alone, b) PP alone, c) PC alone, d) PP + cellulose, e) PC + cellulose, f) PP + PC at 350 °C.

R2 = 0.809

R2 = 0.993

R2 = 0.850



d) PP + Cellulose

R2 = 0.937



e) PC + Cellulose

R2 = 0.888



f) PP + PC

R2 = 0.949

**Discussion regarding interaction effects based on kinetic constants of model:**

Table 1 provides the kinetic constants or k values of the lumped product kinetic model for HTL of unary components – PP alone, PC alone, and cellulose alone. Note that for kinetic values, the absolute values have little physical meaning. Relative values among different reaction pathways help us understand the pathways that are promoted. Also, here we include reversable pathways for the following reaction pathways: components to oil, component to aqueous, oil to aqueous. For these reversible pathways as well, the relative values among the pairs of pathways dictate the rate of reaction.

For HTL of PP alone, we see reaction rates for component to oil, aqueous to oil and component to gas being relatively higher than rest of the reaction pathways. This results in formation of mostly oil and gas products from the initial solid. However, for the reversible reactions, most reverse reactions have a higher rate than the forward reaction, for example, oil to component has a higher rate than component to oil. This means that the forward reaction is not favored. This reasons why so little solid ends up reacting at the first place.

However, the opposite is true for HTL of PC alone. The forward reactions are seen to have a higher rate than the reverse reactions. As a result, higher aqueous, gas and oil yields are obtained from HTL of PC when compared to HTL of PP at 350 °C. Particularly the componentPC --> oilPC reaction rate is high indicating that PC readily liquefies to for oil products at 350 °C. This is understandable since, PC hydrolysis in subcritical water at lower temperatures (250 °C)20. The oil and aqueous products are also seen to readily gasify. Poly bisphenol A carbonate or PC relinks itself using an ester group which is likely decomposing at higher temperatures causing formation of high gas yields. Bisphenol A – the monomeric unit of PC also degrades to form mono-ring phenolic compounds2. Benzene, 1-methoxy-2,4-dimethyl is the main product in GC-elutable oil phase from HTL of PC at 350 °C, 60 mins2. As a result, a methyl groups also gets cleaved from bisphenol A which might again emanate as a gas molecule.

For HTL of cellulose, the reaction rates are completely different from that of the plastics. The initial feedstock component primarily forms aqueous phase products. These aqueous phase further form oil products which further gasify. The rate of reaction for the direct pathway of gasification from the initial feedstock is also high. These observations have been partially made in prior literature. Sheehan et al.10 and Valdez et al12. made similar observations where the cellulose first degrades to aqueous phase and then gets converted to the oil phase. However, previous literature10–13 did not account for direct pathways from cellulose to gas phase.

Table 1: Kinetic constant (k) values for reaction pathways followed by HTL of unary components (PP, PC and cellulose) from lumped product kinetic model. Component in the table refers to the initial feedstock solid that engages the reaction.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | | Kinetic constants for HTL of component i | | |
| Reaction Pathway | Rate equation\* | i = PP | i = PC | i = Cellulose |
| Componenti --> Oili | ri,1=ki,1\*x\_Componenti | 1.11E-03 | 1.80E-01 | 5.15E-03 |
| Oili --> Componenti | ri,2=ki,2\*x\_Oili | 2.33E-02 | 1.75E-03 | 2.16E-02 |
| Componenti --> Aqueousi | ri,3=ki,3\*x\_Componenti | 4.23E-04 | 1.60E-03 | 7.64E-03 |
| Aqueousi --> Componenti | ri,4=ki,4\*x\_Aqueousi | 6.15E-01 | 1.94E-12 | 2.98E-09 |
| Aqueousi --> Oili | ri,5=ki,5\*x\_Aqueousi | 1.37E-01 | 1.16E-04 | 2.53E-01 |
| Oili --> Aqueousi | ri,6=ki,6\*x\_Oili | 1.50E-01 | 3.30E-03 | 7.15E-02 |
| Oili --> Gasi | ri,7=ki,7\*x\_Oili | 6.61E-05 | 1.93E-02 | 1.46E-02 |
| Aqueousi --> Gasi | ri,8=ki,8\*x\_Aqueousi | 6.61E-05 | 3.44E-02 | 6.61E-05 |
| Componenti --> Gasi | ri,9=ki,9\*x\_Componenti | 8.79E-04 | 5.63E-03 | 2.27E-02 |
| Oili --> New solidi | ri,10=ki,10\*x\_Oili | 6.61E-05 | 7.88E-04 | 6.61E-05 |
| Aqueousi --> New solidi | ri,11=ki,11\*x\_Aqueousi | 5.16E-12 | 3.61E-03 | 7.15E-06 |

\*x\_A is the mass fraction of A.

Table 2 gives the kinetic constants of additional pathways which are fit from HTL of binary mixtures. Note that for fitting HTL of PP + cellulose for example, reaction pathways in Table 2 are superimposed on reaction pathways from HTL of PP alone and HTL of cellulose alone, i.e., reaction pathways in Table 1. This enables us to understand the effect of interactions alone i.e., all the additional kinetics that is happening in Table 2 is as a result of interactional effects.

The order of reactions in Table 2 indicates source of increases in oil yield stemming from the interactional effect. The Oilij in the reaction pathway Componenti^a+ Componentj^b --> Oilij is the additional oil formed due to interaction effects. Here, if the order of reaction is higher from one component, that means oil yield increase is happening more from the same component. We observe for HTL of PP + cellulose, the reaction orders are almost equal to each other with a slightly higher value for cellulose. This indicates that the oil yield increase is occurring from both cellulose and PP with a slightly higher fraction coming from cellulose. We further perform quantitative GC/MS analysis in later section to add proof to this observation.

However, for HTL of PC + cellulose and PP + PC, the order of reaction for PP and cellulose are zero. This indicates that the increase in oil yield according to the kinetic model is coming primarily from PC. We can reason this from oil yield observations in previous section where increases in oil yield were occurring primarily for shorter HTL times. Note however, that the model does not fit well for PC + cellulose at longer process times (see Fig. 2). This is because the increases in oil yield from cellulose at longer times is not captured well by the model.

Table 2: Kinetic constant (k) values for reaction pathways followed by HTL of unary components (PP, PC and cellulose) from lumped product kinetic model. Component in the table refers to the initial feedstock solid that engages the reaction.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | | Kinetic constants/ rate orders for binary mixture HTL with component i, component j | | |
| Reaction Pathway | Rate equation\* | i = PP, j = Cellulose | i = PC,  j = Cellulose | i = PP, j = PC |
| a | rij,1=kij,1\* x\_Componentia \* x\_Componentjb | 0.459 | 0.125 | 0.000 |
| b | rij,1=kij,1\* x\_Componentia \* x\_Componentjb | 0.727 | 0.000 | 0.053 |
| Componenti^a+ Componentj^b --> Oilij | rij,1=kij,1\* x\_Componentia \* x\_Componentjb | 4.46E-02 | 1.04E-02 | 2.36E-02 |
| Componenti + Componentj --> Aqueousij | rij,2=kij,2\* x\_Componentia \* x\_Componentjb | 7.96E-04 | 8.49E-03 | 6.04E-05 |
| Aqueousij --> Oilij | rij,3=kij,3\*x\_Aqueousij | 9.14E-01 | 3.00E-06 | 8.39E-03 |
| Oilij --> Aqueousij | rij,4=kij,4\*x\_Oilij | 1.01E+00 | 6.04E-01 | 3.07E-05 |
| Oilij --> Gasij | rij,5=kij,5\*x\_Oilij | 1.82E-02 | 1.09E-01 | 9.84E-07 |
| Aqueousij --> Gasij | rij,6=kij,6\*x\_Aqueousij | 0.00E+00 | 3.29E-06 | 1.88E-08 |
| Componenti + Componentj --> Gasij | rij,7=kij,7\* x\_Componentia \* x\_Componentjb | 3.10E-04 | 7.43E-05 | 5.52E-06 |
| Oilij --> New Solidij | rij,8=kij,8\*x\_Oilij | 2.58E-02 | 1.87E-01 | 1.84E-02 |
| Aqueousij --> New Solidij | rij,9=kij,9\*x\_Aqueousij | 6.26E-17 | 1.02E-01 | 8.62E-03 |

\*x\_A is the mass fraction of A.

From the kinetic constants for HTL of PP + cellulose in Table 2 we see interactions promoting conversion of initial feedstocks to oil phase, conversion of oil to aqueous phase, gasification of oil phase and formation of new solids or char from oil phase. The conversion of initial feedstocks to oil phase has the highest value. As a result, we clearly see increases in oil yields. The reaction pathways promoted here is in line with our previous hypothesis that the hydrogen donation ability of PP alters the reaction pathway of cellulose and that cellulose promotes liquefaction of PP6. The altering of chemical pathways for cellulose leads to shift from production of furans to production of aromatic phenolics. This leads to production of surplus aqueous phase products and char from aromatization of phenolics. We also see from the kinetic model that oil yield increase is also from PP. Thus, the promotion of conversion of initial feedstocks to oil phase is also happening due to enhanced depolymerization of PP.

<Add test experiments that substantiate reason behind oil yield increases – PP + glass beads, cellulose + tetralin, PP + H-deficient chemical>

For HTL of PC + cellulose, conversion of oil to aqueous phase is most promoted followed by reaction pathways for oil to new solids, aqueous to new solids, and oil to gas phase. Thus, we see decreases in oil yields at longer times. This indicates that there is a reversal of pathway from aqueous to oil phase for cellulose as a result of addition of PC. Char formation and gasification pathways are also promoted.

Note that even though the pathway for conversion to oil has lower k values, they are multiplied by two mass fractions which increase their absolute value of the rate. For example, if 0.45, 0.45, 0.05, 0.05 mass fractions are PC feedstock, cellulose feedstock, oil phase and aqueous phase. The rate of reaction for conversion of feedstock to oil and conversion of oil to aqueous would 0.017 and 0.032, respectively. Thus, the conversion of feedstock to oil has a higher rate. <Is this right?>

For the binary plastic mixture for PP + PC, the feedstock to oil, oil to new solids, aqueous to new solids and aqueous to oil reaction pathways are promoted. This results in increase in oil and solid yield. Thus, the kinetic model is fitting well for earlier times when oil yields increase due to synergistic interactions. This leads the kinetic model to have increase in oil yield. The kinetic model does not fit well for longer timelines and hence does not capture the antagonistic interactions.

**Quantitative GCMS analysis of oil phase:**

<GC/MS observation>

**Predictive ability of Kinetic model:**

Fig. 4: Experimental and predicted yields from kinetic for product distributions from HTL of PP + PC + cellulose at 350 °C.



R2 = 0.956  
|R| = 5.53

The kinetic model predicts the product distributions from HTL of equi-mass ternary mixture of PP + PC + cellulose with an average absolute error of 5.53 and R2 value of 0.96. The model equally predicts well for both longer and shorter HTL time scales with average absolute errors of 5.38 and 5.78, respectively. Previous component additivity models that predict oil yields were benchmarked with similar absolute errors6. Seshasayee et al.6 predict oil yields from 141 data points in literature with an average absolute error of 8.20. Note however that this kinetic model can only predict mixtures with PP, PC, and cellulose. This significantly limits the ability to benchmark this model. Since the model fits well, we can say that there are no tertiary interactions between PP, PC and cellulose. <test with adding tertiary interactions to model>

**Conclusion regarding interactional effects:**

<About interactions>

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