

Enhancement of syngas production in co-pyro-gasification of biomass and plastic waste materials: Computational study

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Abstract

The process of co-pyro-gasification of biomass and plastics appears to have the potential for increasing syngas production for power generation and thus minimizing the impact of plastic waste on the environment. This study was based on co-pyro-gasification of selected natural/synthetic polymers and cocoa pod husks as biomass material to ascertain the optimal ratios for enhanced volatile yields. The results showed that gasification of pure biomass commenced at 1500 K, whereas gasification of mixed plastics and biomass started at much lower temperature of 1000 K accompanied with higher syngas yield. Single and multiple plastics produced the most syngas while double plastics had detrimental impact on syngas production. For instance, single plastics with polyethylene terephthalate achieved 65% increase in syngas yield. Mixed-plastics consisting of high-density polyethylene, low-density polyethylene, polypropylene, and polyethylene terephthalate, achieved an increase of 40% - 55% in syngas yield. Whereas antagonistic effects were observed in some double plastics systems such as polyethylene terephthalate and polypropylene. The results indicate that although plastics are instrumental in the thermodynamic equilibrium yields of syngas, the type of plastics and their groupings do also have a significant effect on the yields. Experimental study is recommended to validate the feed proportions for high syngas production.

Keywords: gasification, pyrolysis, pyro-gasification, plastics, cocoa pod husk, cellulose

Introduction

The global energy situation and poor solid waste management effects has prompted the need to explore various biomass and plastic waste resources for power generation especially in developing countries. For instance, Ghana produces over 0.8 million tonnes of cocoa beans annually, representing about 20 % of the world's cocoa beans production, which contributes around one sixth of the country's GDP [1, 2]. The cocoa beans make up about one third of the whole fruit by weight, whilst the cocoa pod husk (CPH), the non-edible lignocellulosic biomass makes up the remainder, and is mainly discarded on the farms. CPH is a rich source of polysaccharides (making up over 60 %) including cellulose, hemicellulose and carbohydrates, aside aromatics and polyphenols. It consists of primarily fibrous materials including 19.7 - 26.1 % cellulose, 8.7 - 12.8 % hemicellulose, 14 - 28 % lignin, 6.0 - 12.6 % pectin, 7 - 10 % proteins, 32 - 47 % carbohydrates, 1.5 - 2 % fats, and minerals (K, Ca and P, Mg, Na, Fe) [3–8].

Reactor controlled biomass partial oxidation for energy via the process of gasification is a much efficient way to trap toxic gases like CO₂ and methane from the combustion of lignocellulosic biomass. Gasification of lignocellulosic biomass produces fuel gas (due to its high volatile content) mainly methane, CO, CO₂ and H₂ for steam and gas generators [9]. The syngas (CO and H₂) can be used to produce electricity but the presence of high amount of CO₂ and tar, do affect the quality and yield of the syngas. In fuel gas production, oxygenated liquid products such as aliphatic liquid hydrocarbons, polyaromatic liquid hydrocarbons, and tar are, formed as by-products as well as char or solid carbon, [9–11] char has useful applications as super capacitor and battery electrodes. Liquids and tar formed under gasification conditions are undesired products as they move along with gases under gasification conditions of temperature and pressure [12–19].

Another waste resource available in abundance globally is plastic, which has become one of the greatest menaces to marine habitats and environmental sustainability across the globe. Most monomers that are used for manufacturing of plastics, are not biodegradable and as a result, they accumulate, rather than decompose, in landfills or in the natural environment. Ghana produces about 3 million metric tonnes of plastic waste annually with only 2 % of these plastic wastes recycled [20]. The bulk of these waste which are from household and have been improperly disposed of, do end up in rivers, lagoons, water channels, the beaches and eventually into the marine coastal environment. Due to dysfunctional waste management services, some wastes containing high plastic content are regularly burned in the open, thus releasing highly toxic substances such as dioxins and furans into the environment. According to the World Health Organization (WHO), this is a major source of air pollution, which contributes to about 28,000 premature deaths in Ghana every year [20].

Numerous studies have shown that mixed plastics waste can be gasified to produce syngas for electricity generation but there are issues with corrosive and toxic components such as tar production, which do affect the quality and yield of the syngas [9, 12, 16, 21-22]. However, a comprehensive review conducted by Block et al. [23] showed that those effects could be minimized through co-pyrogasification of plastics and biomass. For instance, Pinto et al [24] co-gasified biomass mixed with 60 % (w/w) plastic in feedstock and achieved a reduction in tar and an increase in H₂ and in the overall gas content by 98%. Plastics from municipal solid waste, automotive shredder residues, polyethylene (PE) regrind, and virgin PE were also co-gasified with biomass and achieved considerable reduction in tar content [25]. Although these studies [21, 24, 25] have shown the potential of plastics to improve on the purity of syngas, there is the need for the gasification process to be optimized, to achieve the desired product distribution or syngas

composition, through operating parameters such as reactor temperature, equivalence ratio (air or oxygen), steam/fuel ratio and catalyst. This study was therefore focused on investigating the properties of the commonly available plastics waste in Ghana such as high-density polyethylene (H), low-density polyethylene (L), polypropylene (PP) and polyethylene terephthalate (P) and their effects on process optimization for gasification of CPH.

2.0 Numerical modelling approach

Understanding the role of multi-plastics in the gasification of biomass at molecular level is necessary to enable effective control of desired product composition. To this end molecular dynamics (MD) simulation approach was used to study the thermodynamic properties and to establish the optimal feed proportion of the plastics for high syngas production. It does enable the motions and trajectories of the molecules to be investigated during a transformation under certain thermodynamic conditions and state variables of T, P, V, and n. In MD, atoms with initial positions and velocities are exposed to motions governed by the empirical interatomic potentials (EIP) based on time. Before carrying out MD simulation, information is required about the geometry (type of atoms, bond angles, lengths, etc.) initial positions (r), velocity (v), charge (q) and force fields.

The reactive force-field (ReaxFF) interatomic potential is a powerful computational tool for exploring interactions at interfaces as it considers bond-order formalization as well as the empirical interatomic potential that reduces computational cost [40]. Initial geometries of biomass polysaccharide i.e., cellulose (C), was built from 40 units of 14bD-glucose with β -1,4- glycosidic bond linkages. Units of polypropylene (PP), polyethylene terephthalate (P), low-density polyethylene (L), high-density polyethylene (H) were constructed from their monomer units of isotactic propylene, isotactic ethylene terephthalate, isotactic ethylene and atactic 1-butene to

represent polymer to biomass percentage weight-by-weight (w/w) ratios as reported in **Table 1**. In all discussions, C represents cellulose, P represents PET, H represents HDPE, L represents LDPE and PP represents PP in polymer mixtures. Hence, CP is cellulose with PET, CPP is cellulose with PP, and CPPP is cellulose with PET and PP etc. Trimers of the building monomers are shown in **Fig 1**, for cellulose (a), polyethylene terephthalate (b), polypropylene (c), high-density polyethylene (d) and low-density polyethylene (e).

Pyro-gasification is a thermal treatment, which involves the following steps: drying, pyrolysis or devolatilization, char gasification, and (partial) oxidation. Pyrolysis occurs in the absence of oxygen gas at temperatures between 300 and 800°C. While gasification of char starts later at 500 to 1500 °C, in the presence of a gasifying agent like air, pure oxygen, steam, carbon dioxide or a combination thereof, which can be generated within. Pyrolysis leading to gasification has been simulated at temperatures of 1000 K (~700 °C), 1500 K (~1200 °C) and 2000 K (~1700 °C). Both processes lead to the production of solids (mostly char), liquids (tars, heavy hydrocarbons, oil) and gases (CO₂, H₂O, CO, C₂H₂, C₂H₄, C₂H₆ etc.). In this study the products have been classified as follows; gases as C₁₋₄ compounds, bio-oils as C₅₋₁₉ compounds, tar as C₂₀₋₄₅ compounds and solid char as > C₋₄₅ compounds.

The ReaxFF force fields [26] were employed as implemented in the LAMMPS molecular dynamics package [27]. Structures were minimized to their ground state structure at absolute zero temperature of 0 K where velocity is 0 ms⁻¹ and translational motions are absent. The system was heated gradually, first heated to room temperature of 300 K using the NVE microcanonical ensemble where velocity was introduced to the frozen atoms for 2000 fs or 2 ps. Subsequently, the system was equilibrated at the desired reaction temperatures (i.e., 1000 K, 1500 K and 2000 K.) for 5000 fs or 5 ps at each temperature. The canonical (NVT) ensemble was used in all co-pyrolysis

models representing a closed system. In the isochoric and isothermal system adopted, heat exchanges and pressure variations were possible, as energy and pressure were not fixed during the reaction process. The Berendsen thermostat was used to control temperatures with a damping constant of 1 fs. The atomic motions were updated and summarized by velocity Verlet algorithm with a 0.1 fs time-step. All trajectories and structures were visualized with the Ovito software [28] and Vesta software [29].

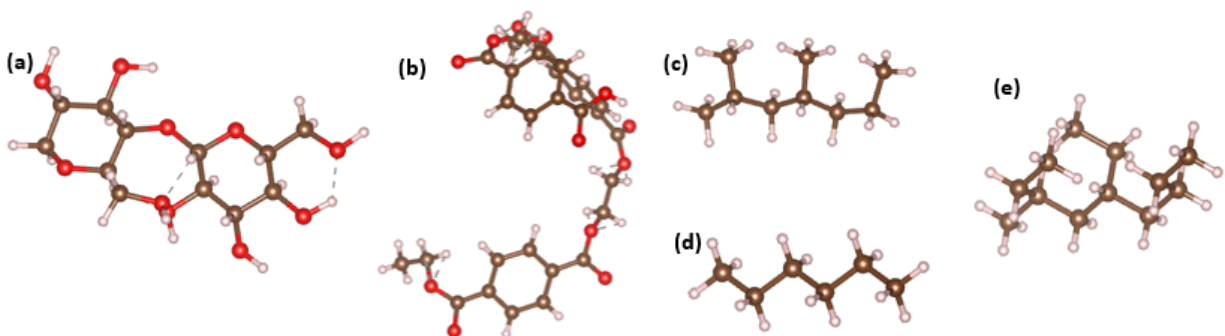


Fig. 1 Trimers of building units i.e., 14bD glucose (a), ethyl terephthalate (b), propylene (c), ethylene (d) and 1-butene (e)

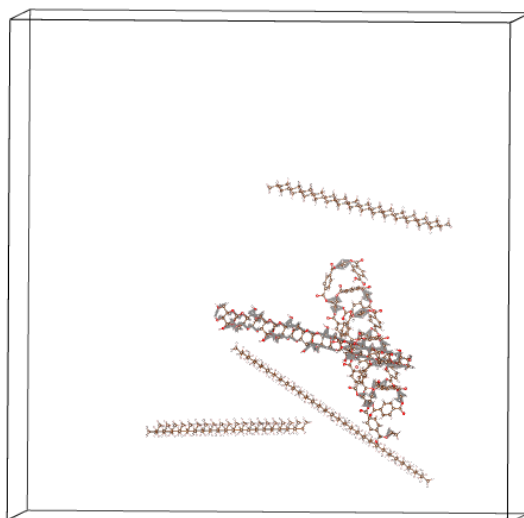


Fig. 2 Sample simulation cell of CPPPHL with 40 units of cellulose chain with plastics (i.e., PP, PET, HDPE, LDPE) in a 200 x 200 x 200 Å³ box

3.0 Results and discussions

3.1 System calibration

Using 40 units of cellulose and reaction time of 80,000 fs, an initial system calibration was carried out to ascertain the time required for the system to attain equilibrium. From **Fig 3**, the system equilibrates after 60,000 fs as the total energy of the system is not lowered any further, and there is no further macroscopic change as chemical composition is stabilized. Hence, in all simulations product yields in the vessel are quantified and compared after 60,000 fs.

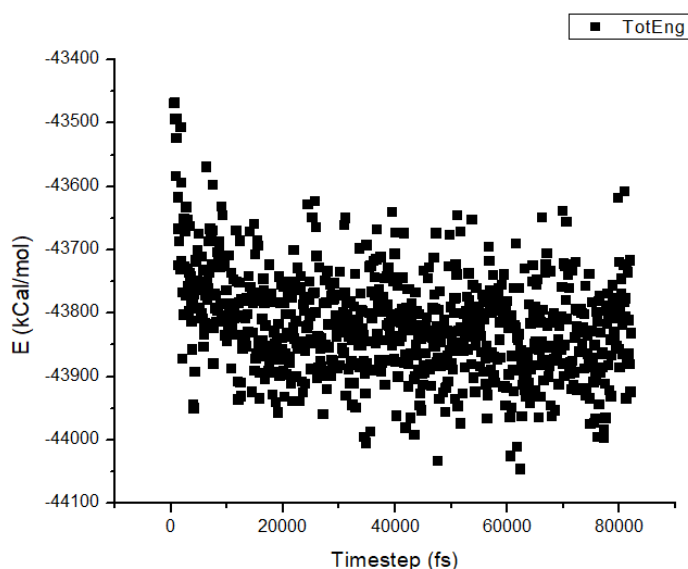


Fig. 3: Method calibration plot with the Berendsen thermostat

3.2 Volatile products from Biomass/ Plastics (PP, HDPE, LDPE and PET) Mixtures

Pyro-gasification of cellulose-plastic mixtures were considered at three different temperatures: the pyrolysis temperature of 1000 K, gasification temperature of 1500 K and extreme temperature degradation of 2000 K. As shown in **Fig 4a**, cellulose gasification was initiated at 1500 K and gasification temperature was lowered to 1000 K for all plastic modified cellulose (except in the case of CH, CPPL, CPPPL, CPLH). At 1500 K, the gases produced were increased from 40 % for

cellulose to as high as 65 % for cellulose with polyethylene terephthalate. Gas yields were generally increased in most plastic composites, especially for the single plastic systems in the order of CP > CH > CL > CPP. The amount of gas yields from CH alone was comparable to the gas produced from the mixed plastic system (i.e., cellulose + P + H + L + PP) of 55 %. Some double (CPPP, CPL, CPH, CPPH and CPPL) and triple (CPPLH and CPPPH) plastics had detrimental effects on the volatile content of biomass as gas yields were lowered. Although the triple plastic systems (CPPLH and CPPPH) did not produce appreciable carbon gases, they produced the most hydrogen species. Tar product was reduced in most cases but was increased in double plastic systems i.e., CPPL and CPPP composites. For multi-plastic systems, where all 4-plastic types are present forming a 5-component system, gas amounts greater than cellulose was observed, with lowered tar and char yields. These results show that antagonistic effects are more pronounced in double plastic systems. However, in single plastics and multi-plastic composites, the activity of the cellulose is improved, leading to high gas yields and lower high-density liquid formation. The multi-plastic system is attractive, as it does not involve the cost of plastic sorting prior to gasification.

At the pyrolysis temperature of 1000 K, cellulose selectively produced 60% bio-oils, 20 % tar and 20 % char. Plastic mixed cellulose reduced bio-oils to about 20 % and tar to 10 %, whereas char increased to near 40 % – 60 %. Plastics also produced some gases ranging from 20 – 50 % at a temperature of 1000 K. The results indicate that although plastics are instrumental in the thermodynamic equilibrium yields of syngas, the type of plastics and their groupings do also have a significant effect on the yields. For example in **Fig 4c**, polyethylene terephthalate systems did lower the gas production in the CPPP (20 %), CPL (25 %) and CPH (20 %) composites. However, multiplastics with polyethylene terephthalate (CPPPLH = 55 %) and single plastics with

polyethylene terephthalate (CP = 65 %) reduced this effect and produced high gas yields as compared to cellulose (C = 40 %).

3.3 Plastic Amount Variation Effects on Volatile Yields

After identifying the most efficient groupings of plastics, the effect of plastic ratios on pyrolysis and gasified products were also studied. At 1500 K, it was observed that, by increasing the plastic concentration from 20 % (as discussed in earlier sections) to 40 %, the gaseous products were further increased from 55 % to about 65 % (see **Fig. 5** and **Table 2**). The hydrogen species was however, not altered by the increase in plastic amount. Liquids production levels were reduced at 40 % plastic composition as compared with 20 % and 30 %. For instance, liquids levels were lowered from 20 % to 15 % in pure cellulose with 40 % plastics. In all, 40% plastic composition was seen as an efficient combination as it did decrease liquid, char and tar formation as compared to the other combinations. On the other hand 10% plastic composition was also found to be desirable since in comparison with 40 % plastic, the tar and liquid were significantly eliminated and char was selectively produced as byproduct.

To reduce reaction energies, increase yields, and to reduce byproduct formation, strategies of plastic mix aside catalysis is seen in the current study as an effective approach to achieve a selective production of pyrolysis and gasification products. The lower energies required for decomposing cellulose suggests the possible activation of cellulose by the presence of the plastics leading to its ease of decomposition and lower energy requirements for bond dissociations. The equilibrium structures of the various polymer composites at different temperatures are provided as supplementary information in **Fig. S1, S2, S3** and **S4**.

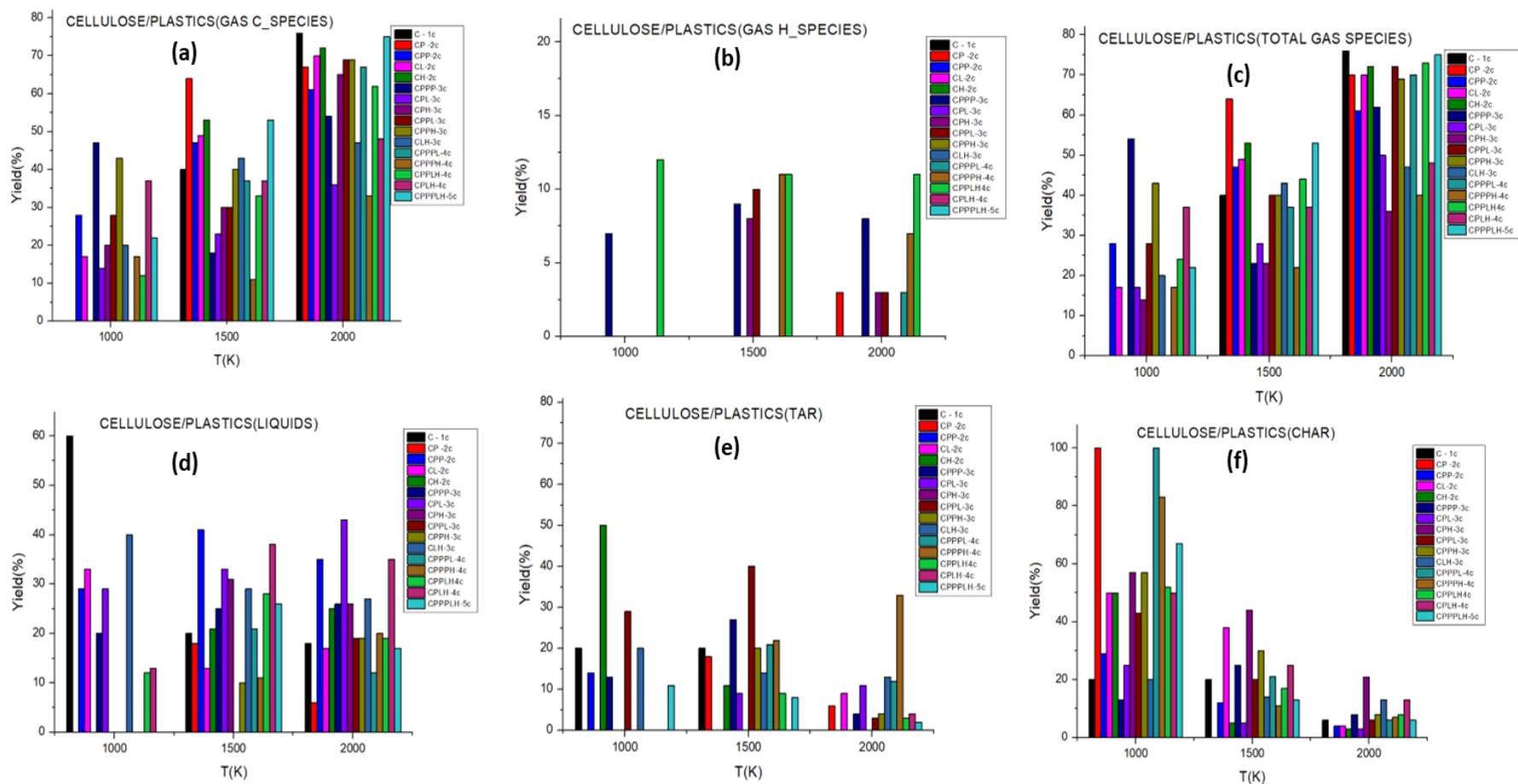


Fig. 4 Graphical summary of thermal product yields of the co-pyrogasification of cellulose and plastics (with P, PP, H and L), under pyrolysis temperature (1000 K), gasification temperature (1500 K) and extreme temperature (2000 K)

Table 1: Summary of thermal product yields of the co-pyrogasification of cellulose and plastics (with P, PP, H and L), under pyrolysis temperature (1000 K), gasification temperature (1500 K) and extreme temperature (2000 K)

T/K	C - 1c 0%	CP -2c 5%	CPP -2c 5%	CL -2c 5%	CH -2c 5%	CPPP -3c 10%	CPL -3c 10%	CPH -3c 10%	CPPL -3c 10%	CPPH -3c 10%	CLH -3c 10%	CPPPL -4c 15%	CPPPH -4c 15%	CPPLH -4c 15%	CPLH -4c 15%	CPPPLH -5c 20%
C1-4 GASES																
1000	0	0	28	17	0	47	14	20	28	43	20	0	17	12	37	22
1500	40	64	47	49	53	18	23	30	30	40	43	37	11	33	37	53
2000	76	67	61	70	72	54	36	65	69	69	47	67	33	62	48	75
H GASES																
1000	0	0	0	0	0	7	0	0	0	0	0	0	0	12	0	0
1500	0	0	0	0	0	9	0	8	10	0	0	0	11	11	0	0
2000	0	3	0	0	0	8	0	3	3	0	0	3	7	11	0	0
C5-19 LIQUIDS																
1000	60	0	29	33	0	20	29	0	0	0	40	0	0	12	13	0
1500	20	18	41	13	21	25	33	31	0	10	29	21	11	28	38	26
2000	18	6	35	17	25	26	43	26	19	19	27	12	20	19	35	17
C20-45 TAR																
1000	20	0	14	0	50	13	0	0	29	0	20	0	0	0	0	11
1500	20	18	0	0	11	27	9	0	40	20	14	21	22	9	0	8
2000	0	6	0	9	0	4	11	0	3	4	13	12	33	3	4	2
C>45 CHAR																
1000	20	100	29	50	50	13	25	57	43	57	20	100	83	52	50	67
1500	20	0	12	38	5	25	5	44	20	30	14	21	11	17	25	13
2000	6	0	4	4	3	8	3	21	6	8	13	6	7	8	13	6

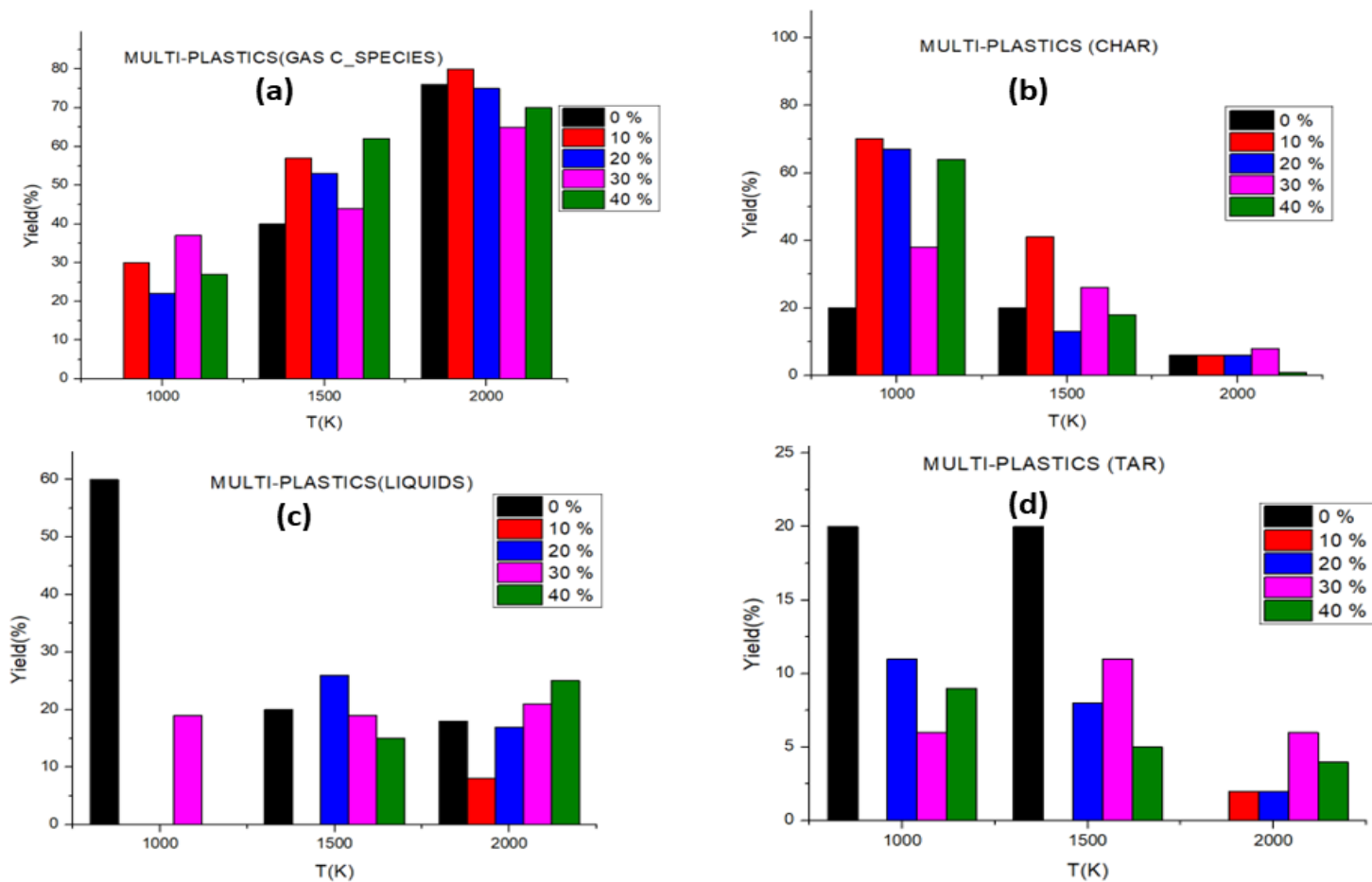


Fig. 5 Pyrogasification yields of varying percentage w/w ratios of mixed plastics with cellulose, under pyrolysis temperature (1000 K), gasification temperature (1500 K) and extreme temperature (2000 K)

Table 2: Pyro-gasification yields of varying percentage w/w ratios of mixed plastics with cellulose, under pyrolysis temperature (1000 K), gasification temperature (1500 K) and extreme temperature (2000 K)

T/K	10%	20%	30%	40%
C1-4 GASES				
1000	30	22	37	27
1500	57	53	44	62
2000	80	75	65	70
H GASES				
1000	0	0	0	0
1500	0	0	0	0
2000	0	0	0	0
C5-19 LIQUIDS				
1000	0	0	19	0
1500	0	26	19	15
2000	12	17	21	25
C20-45 TAR				
1000	0	11	6	9
1500	0	8	11	5
2000	2	3	6	4
C>45 CHAR				
1000	70	67	38	64
1500	41	13	26	18
2000	6	6	8	1

4.0 Conclusions

In this study, the yields of co-pyro-gasification of plastics and cellulose were considered, using different combinations of plastics at both pyrolysis and gasification temperatures. The results showed that most of the plastics did enhance the yields of syngas and increased char products while reducing tar and liquids. The specific outcomes could therefore be summarized as follows:

- Single plastics and multiple plastics produced the most syngas while double plastics consisting of polyethylene terephthalate and polypropylene had detrimental impact on syngas production.

- Co-pyro-gasification of cellulose and 40% of mixed plastics (P, PP, H and L), achieved the highest gas yield increase of 40 % to 55 %.

Above all, the study has shown that the use of mixed plastics has some added economic benefit, as multi-plastic gasification does not involve cost implications of sorting out plastics from different sources. Extensive experimental evaluation is being recommended to establish the true potential of these plastics for power generation.

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Supporting Information

Figures S1, S2, S3 and S4 show the geometries obtained at different energies.

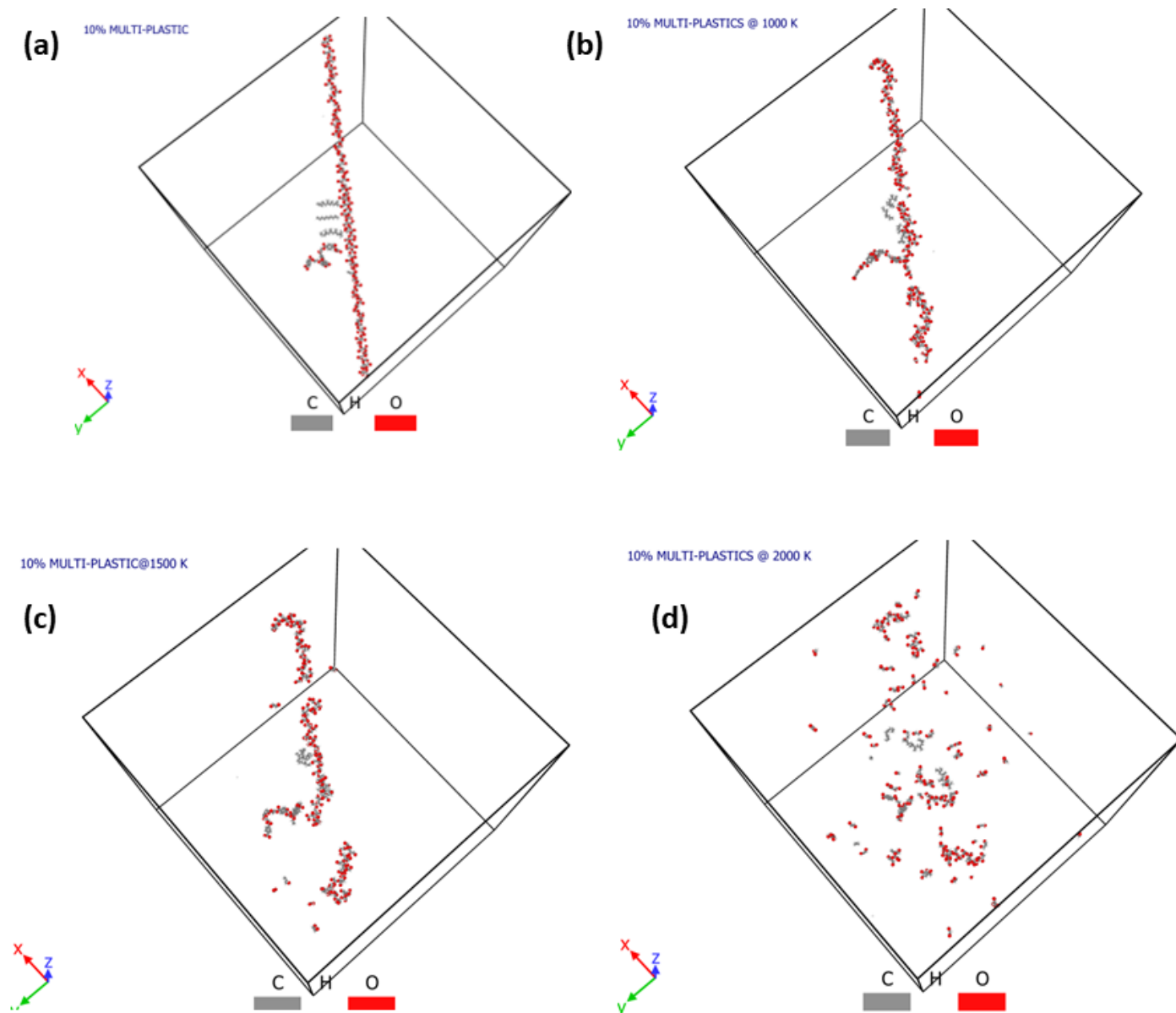


Fig. S1 Equilibrium geometries of 10 % Plastics (PP, HDPE, LDPE, and PET) mixed with cellulose at 300 K (a), 1000 K (b), 1500 (c), 2000 (d)

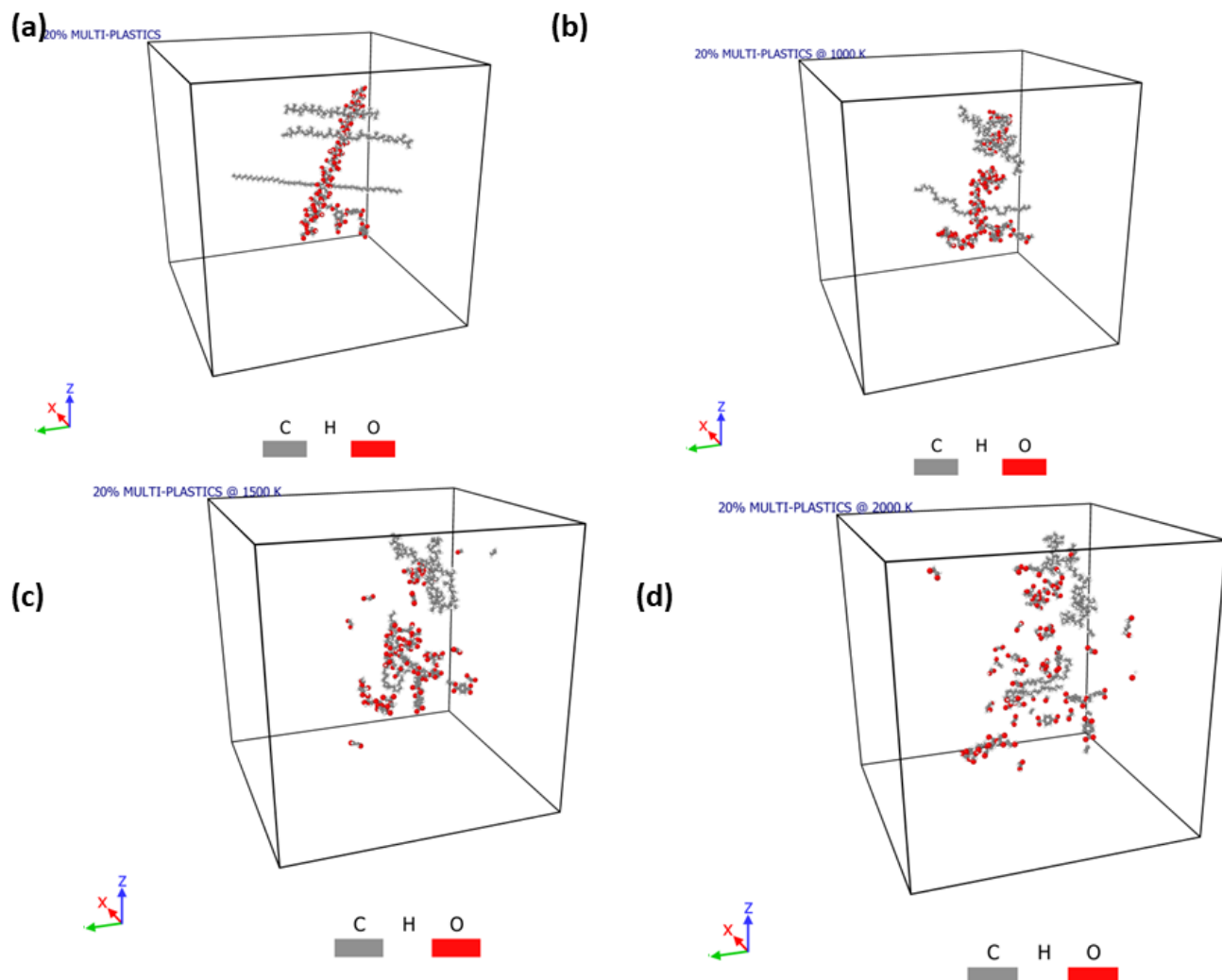


Fig. S2 Equilibrium geometries of 20 % Plastics (PP, HDPE, LDPE, and PET) mixed with cellulose at 300 K (a), 1000 K (b), 1500 (c), 2000 (d)

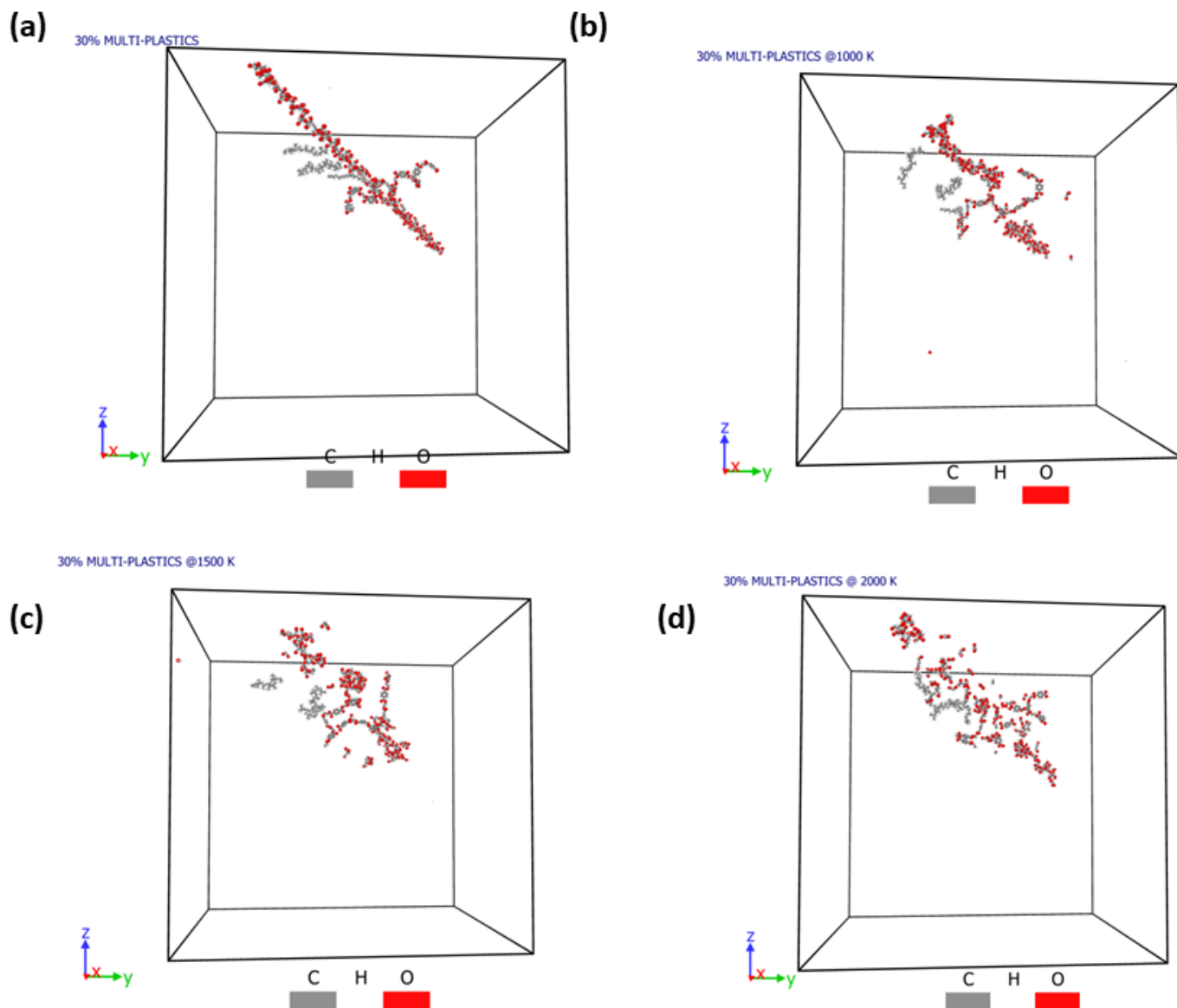


Fig. S3 Equilibrium geometries of 30 % Plastics (PP, HDPE, LDPE, and PET) mixed with cellulose at 300 K (a), 1000 K (b), 1500 (c), 2000 (d)

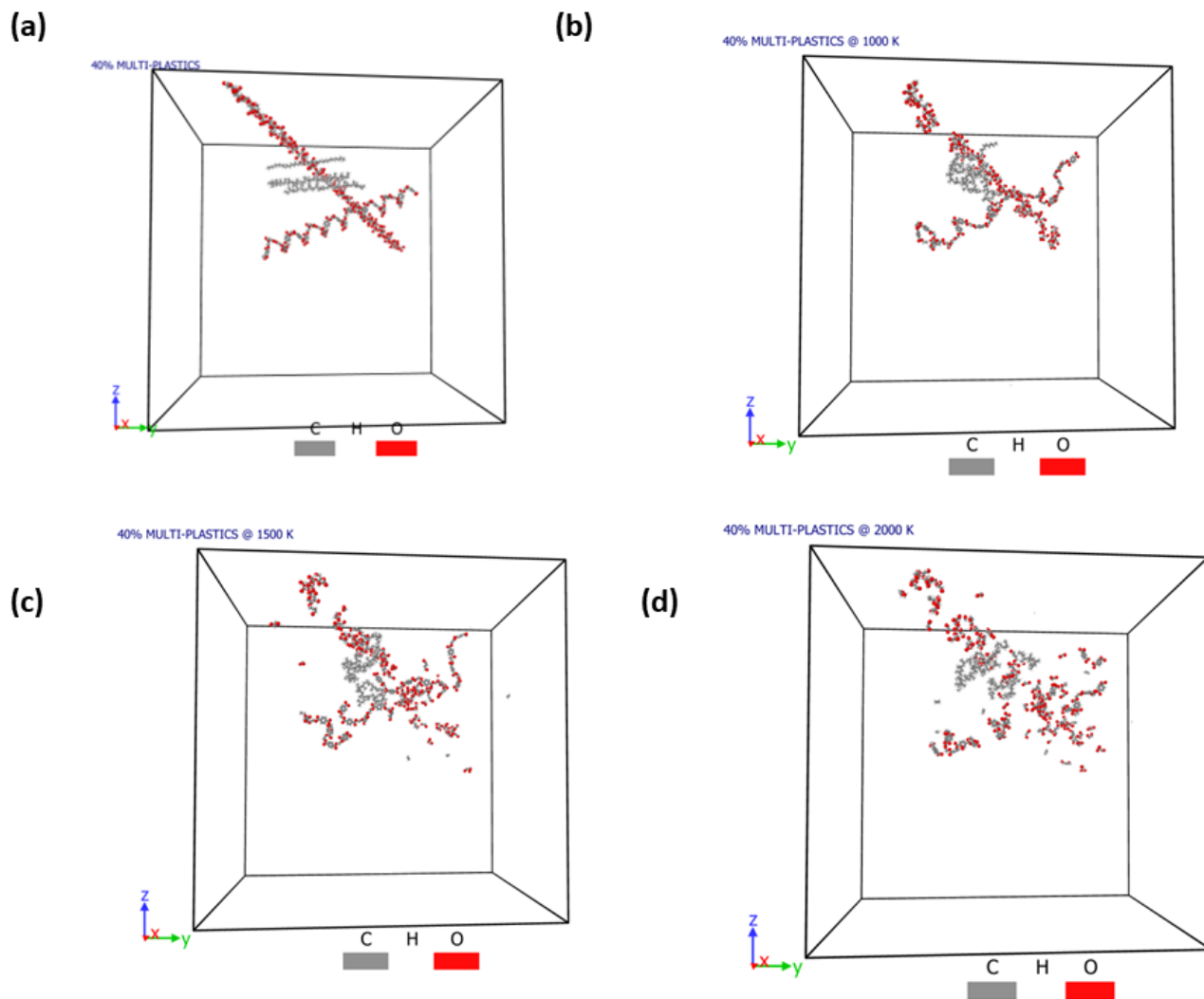


Fig. S4 Equilibrium geometries of 40 % Plastics (PP, HDPE, LDPE, and PET) mixed with cellulose at 300 K (a), 1000 K (b), 1500 (c), 2000 (d)