Supplementary information

Feedstock agnostic upcycling of industrial mixed plastic from shredder residue pragmatically through a composite approach

Kanjanawadee Singkronart[§], Andre Gaduan[§], Siti Rosminah Shamsuddin[§], Keeran Ward[¢], Koon-Yang Lee[§,†,*]

[§]Department of Aeronautics and [†]Institute for Molecular Science and Engineering (IMSE), Imperial College London, London, SW7 2AZ, United Kingdom. [¢]School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT, United Kingdom.

[*]Corresponding author (KYL). Email: koonyang.lee@imperial.ac.uk; Tel: +44 (0)20 7594 5150

Table of content

S1: Steam gasification of industrial mixed plastic from shredder residue

The process model (Fig. S1) gives an overview of a combined cycle power generation plant utilising waste plastics gasification. The model is developed and validated in accordance with the works from Saebea et al. (Energy Reports 2020 6, 202-207) and Salah et al. (ACS Sustainable Chem. Eng. 2023, 11, 3238–3247). The process was modelled in Aspen Plus V10, using the RK-SOAVE thermodynamic property package, employing the Redlich-Kwong-Soave cubic equation of state- suitable for predicting the properties of hydrocarbon mixtures at high temperatures and pressures (ACS Sustainable Chem. Eng. 2023, 11, 3238–3247). The feedstock (25^{o}C, 1 bar), comprising a mixture of 50 wt% acrylonitrile butadiene styrene (ABS), 40 wt% polystyrene (PS) and 10 wt% polypropylene (PP), was mixed with saturated low pressure (LP) steam (6 bar) in a mass ratio of 1:1.5 (plastic: steam), and fed to a gasification unit operating at 800^{o}C and 1 bar. The gasification process was modelled using a Yield reactor (D-101) and a Gibbs reactor (GASIFIER), where synthesis gas (CO, H_2, CO_2, CH_4, N_2) was produced from the chemical transformation of waste plastics. D-101 facilitates the decomposition of the plastics into C, H_2 and N_2, utilizing mass balances guided by the feedstock elemental composition provided in Table S1, while the GASIFIER operates by predicting the mass flows of the synthesis gas based on Gibbs Free Energy minimization. The subsequent synthesis gas was combusted with excess air producing flue gas, which was routed to a combined cycle power generation unit comprising a Brayton cycle using a gas turbine (G-TR), and a Rankine cycle utilizing heat recovery steam generation (HRSG) - involving saturated/superheated steam heat exchangers (HX3/HX2 respectively) and two steam turbines operating at 100 bar (HP) and 6 bar (LP). The exhaust steam was condensed (COND1), pumped to 100 bar (BFWPUMP) and recycled to the HRSG unit. Additionally, heat was recovered from cooling hot effluent synthesis gas facilitating LP steam production (HX1) as well as integrating thermal heat from combustion (R-101) into gasification. Ultimately, the thermal efficiency of the process was estimated to be 44% (Table S2) - in alignment with common gasification processes (Energy Conversion and Management 2015, 105, 530-544).

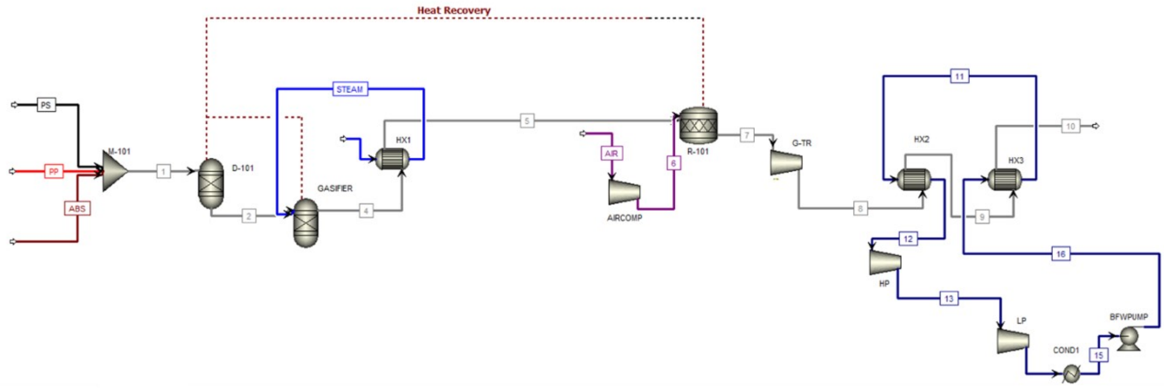

Figure S1: Process flow diagram of waste plastics gasification and power generation.

Table S1: Chemical characterisation of industrial mixed plastic from shredder residue for use in the process model in Fig. S1.

Proximate Analysis[a] (wt%)	ABS	PS	PP
Carbon	-	-	-
Volatiles	100	100	100
Ash	-	-	-
Moisture	-	-	-
Elemental Analysis (wt%)			
C	85.36	92.31	85.71
H	8.04	7.69	14.29
N	6.60	-	-
S	-	-	-

[a]Ash, moisture and sulphur composition was assumed to be negligible for this study.

Table S2: Power generation system inventory normalised to 1 kg of industrial mixed plastic from shredder residue.

Material/Energy flow	Amount
INPUTS	
Waste Plastics [kg/kg]	1.0
Water [kg/kg]	1.5
Electrical energy [kWh/kg]	2.68
Cooling load [MWh/kg]	0.002
OUTPUTS	
Electrical energy [kWh/kg]	6.63
CO_2 [kg/kg]	3.23
Energy Balance	
Feedstock Calorific Value* [MWh/kg]	0.00896
Net Electrical Energy [MWh/kg]	0.00395
Efficiency [%]	44.0

*Maksimuk et al. Fuel 2020, 263, 116727.

S2: Mesh convergence of our chair model in Abaqus

The simulation results of a chair model in Fig. 3 of virgin PP are collected and the mesh sensitivity study is shown in Fig S3. It shows the deflection and stress result converged at 14.37 mm and 12.43, respectively, at which 199,317 elements.

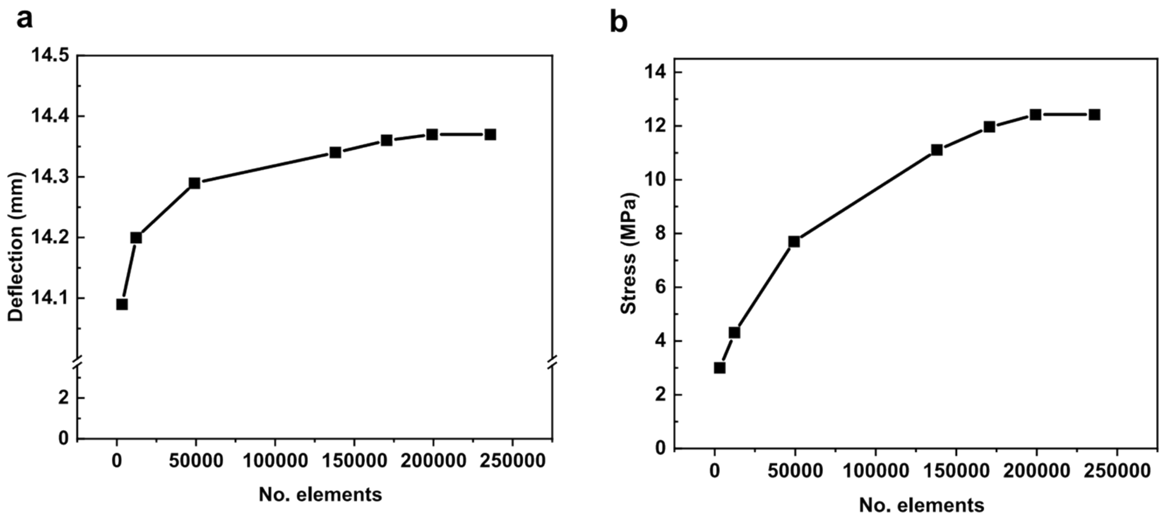

Figure S2. (a) deflection and (b) stress sentivity study on number of elements

S3: Life-cycle inventory of processes considered in the LCA

Inventory	**GWP (-credit) kg CO_2-eq.**	**ADP (-credit) MJ**	**Reference**
Production of 1 kg ABS	3.11	81.4	Gabi Professional
Production of 1 kg PS	2.24	74.7	Gabi Professional
Production of 1 kg PP	1.63	71	Gabi Professional
Production of 1 kg talc	0.29	3.49	Gabi Professional
Production of 1 kg GF	1.7	22.2	Gabi Professional
Production of 1 kg CF	14.60	454	Meng et al., 2017
Forestation of 1 kg spruce wood	-1	0.28	Gabi Professional
Grinding 1 kg of spruce wood	0.26	3.52	Repellin et al., 2010
Use phase 1 kg panel	20.75	250	Gabi Professional
Recovery 1 kg of mixed plastic	0.35	4.75	Ciacci et al., 2010
Landfill 1 kg of plastic waste	1.02	0.743	Gabi Professional
Incineration 1 kg of plastic	0.85	-19.85	Gabi Professional
Incineration 1 kg of wood waste	1.21	-19.45	Gabi Professional
Petroleum production 1 kg (GB)	0.56	48	Gabi Professional
Electricity grid 1 kWh (GB)	0.321	4.4	Gabi Professional

S4: Exemplary calculation to determine the mass of the f.u.

In this example, we used the mechanical properties of 40 wt.-% CF-reinforced mixed plastic as the model material.

In tension:

Tensile yield strength $(\sigma^{Yield}_{Tensile})$ = 31 MPa @ 0.14%

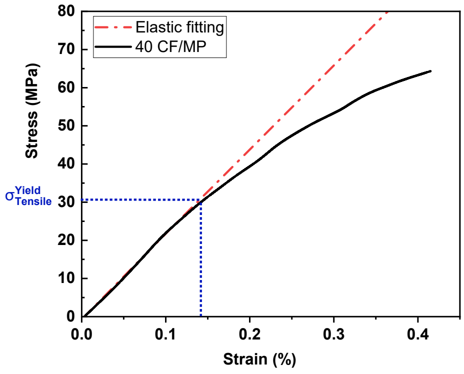

Fig S3. Elastic fitting for tensile yield strength

In bending:

Flexural yield strength $(\sigma^{Yield}_{Flexural})$ = 74 MPa @ 0.42%

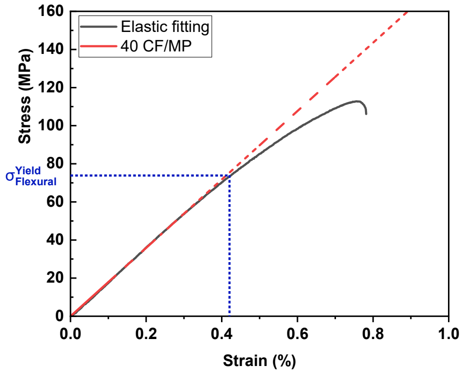

Fig S4. Elastic fitting for flexural yield strength

In fracture:

From section 3.5, K_{IC} of 40 wt.-% CF-reinforced MP was found to be 2.61 MPa $m^{0.5}$. Assuming the existence of a crack in an infinite plate and in the worst case scenario, the crack possesses the same dimension as the diameter of the CFs (7 µm), $\sigma_{Fracture}$ is calculated as:

$$\sigma_{Fracture} = \frac{K_{IC}}{\sqrt{\pi a}} = \frac{2.61}{\sqrt{\pi \times 7 \times 10^{-6}}} = 556.6\ MPa$$

Based on these, the design stress for 40 wt.-% CF-reinforced MP is the smallest of the 3 stresses, which is **31 MPa.**

S5: Mass of functional unit of PP, WF-reinforced, GF-reinforced and CF-reinforced residual mixed plastic (MP) with FEA and E-driven beam bending design

Materials	Mass of f.u. based on FEA design (kg)	Mass of f.u. based on E-driven beam bending design (kg)
PP	3.47 ± 0.31	
MPs	3.41 ± 0.17	3.70 ± 0.04
WF/MP (wt.%)		
2.5	3.51 ± 0.04	3.60 ± 0.06
5	3.67 ± 0.15	3.63 ± 0.04
10	3.74 ± 0.11	3.57 ± 0.04
20	3.73 ± 0.22	3.40 ± 0.03
40	3.69 ± 0.15	3.02 ± 0.04
GF/MP (wt.%)		
2.5	3.50 ± 0.07	3.62 ± 0.04
5	3.51 ± 0.07	3.47 ± 0.04
10	3.63 ± 0.04	3.44 ± 0.03
20	3.62 ± 0.25	3.26 ± 0.04
40	3.93 ± 0.31	3.19 ± 0.05
CF/MP (wt.%)		
2.5	3.49 ± 0.25	3.31 ± 0.05
5	3.27 ± 0.20	3.09 ± 0.06
10	3.19 ± 0.13	2.78 ± 0.12
20	2.98 ± 0.30	2.58 ± 0.11
40	3.08 ± 0.34	2.43 ± 0.11