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Data Article

Evaluation of synergy during co-pyrolysis of torrefied sawdust, coal and paraffin. A kinetic and thermodynamic dataset

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ABSTRACT

This article aims to clarify and expand the information published in the article *Evaluation of synergy during co-pyrolysis of torrefied sawdust, coal and paraffin. A kinetic and thermodynamic study*, which evaluate kinetically and thermodynamically the existence of synergies during the co-pyrolysis of binary and ternary blends of coal, torrefied pine sawdust and paraffin. These materials were selected because they have been used before in the preparation of briquettes for the steel industry with good results. In order to facilitate the understanding and reproducibility of the main article, the following descriptions, dataset and figures have been provided: description and formulation of iso-conversional methods, some TGA curves and the standard deviation of the TG analysis, the activation energy of all the raw materials and their blends at different level of conversion using Friedman, Kissinger-Akahira-Sunose (KAS) and Flynn-Wall-Ozawa (FWO) methods, as well as, the linear plots for their calculations for the KAS and FWO models; also the thermodynamic parameters for pyrolysis of all the samples studied and the theoretical and experimental plots for prediction of solid state reaction mechanism using Criado method of several weights of paraffin are include.

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Specifications Table

Subject	Environmental Science
Specific subject area	Environmental Engineering
Type of data	Tables and figures.
How data were acquired	Thermogravimetric analysis (TGA) was carried out in a TA Instruments SDT 2960 thermoanalyzer.
Data format	Raw
Parameters for data collection	Samples with a particle size of <0.212 mm were used for each pyrolysis experiment. The samples were pyrolyzed from room temperature to 1000 °C, at 3, 10, 20, and 40 °C/min. Nitrogen was used to maintain an inert atmosphere at a flow rate of 100 mL/min.
Description of data collection	Thermogravimetric analysis data were collected: mass loss and temperature.
Data source location	The thermogravimetric analysis data were collected at Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, Oviedo, Asturias, Spain. https://data.mendeley.com/datasets/w22346frww/2
Data accessibility	With the article
Related research article	L. Florentino-Madiedo, M.F. Vega, E. Díaz-Faes, C. Barriocanal, Evaluation of synergy during co-pyrolysis of torrefied sawdust, coal and paraffin. A kinetic and thermodynamic study, Fuel 292 (2021) 120305. https://doi.org/10.1016/j.fuel.2021.120305 [1]

Value of the Data

- Information on this data article deeply contributes to the understanding of thermochemical conversion processes. It described kinetically and thermodynamically the interactions of materials that have not been studied before.
- Researchers in environmental engineering, material sciences, chemical, energy and related areas may benefit from the data presented in this work.
- The data describe in deep how the initial mass and heating rate affect the paraffin thermochemical decomposition. In addition, data of kinetic and thermodynamic parameters of pyrolysis of coal, torrefied sawdust and paraffin, as well as their blends, at different level of conversion is presented here.
- This data set will be beneficial for researchers who want to develop experiments with any of the material studied at this article or related materials. Also, these results contribute to the industry by describing new ways to reduce the energy required to carry out thermochemical conversion processes.

1. Data Description

This article contains supplementary material for the paper *Evaluation of synergy during co-pyrolysis of torrefied sawdust, coal and paraffin. A kinetic and thermodynamic study.* Section 2, presents, in detail, the descriptions and formulation of the iso-conversional methods used. The TGA data of paraffin thermochemical decomposition is presented in Fig. 1. Table 1 shows the values of maximum standard deviations of the experimental and calculated DTG curves. Figs. 2 and 3 shows the linear plots corresponding to the calculation of the activation energy (Ea) of the raw materials, using KAS and FWO methods. The linear plots of the blends studied, i.e. SPT/P, C/SPT, C/P and C/SPT/P, using KAS and FWO models, are presented in Figs. 4 and 5 . The linear plots calculated by Friedman model are presented at the main article. The Ea values at different

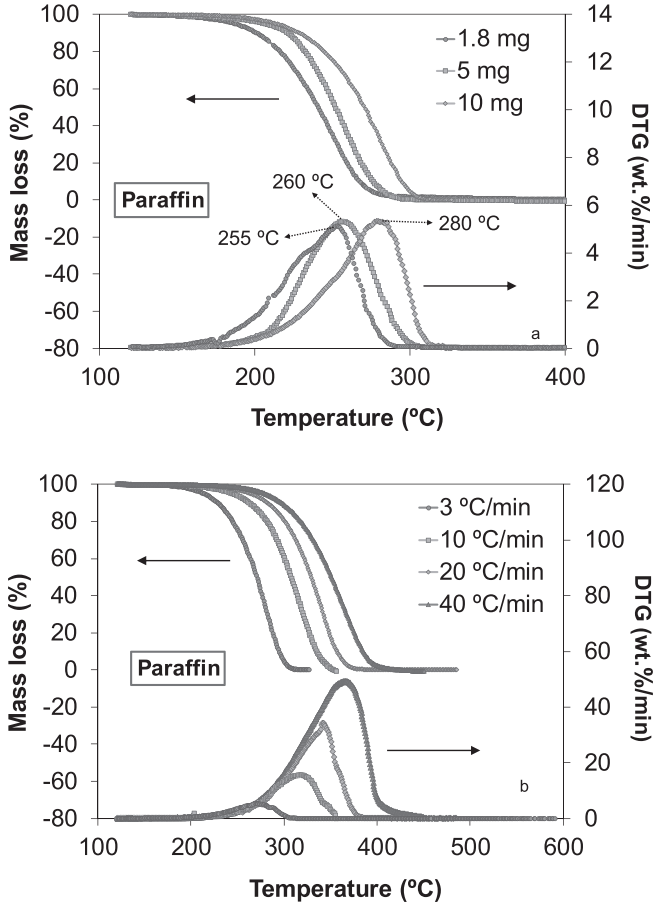

Fig. 1. TGA analysis: (a) TGA curves of paraffin for different initial weights at heating rate 3°C/min and (b) TGA curves of paraffin at different heating rates.

Table 1
Values of maximum standard deviations of two replicas of the experimental DTG curves (DesMax-EXP/EXP) and of the experimental DTG curve and the calculated one (DesMax-EXP/CAL).

Heating Rate	Samples	DesMax EXP/EXP	DesMax EXP/CAL
3 °C/min	C/SPT	0.10	0.07
	C/P	0.16	0.16
	C/SPT/P	0.14	0.15
	SPT/P	0.19	1.20
10 °C/min	C/SPT	0.42	0.51
	C/P	1.13	0.63
	C/SPT/P	0.43	0.42
	SPT/P	0.67	2.79
20 °C/min	C/SPT	1.58	1.58
	C/P	0.84	0.82
	C/SPT/P	0.42	1.21
	SPT/P	0.94	4.29
40 °C/min	C/SPT	1.38	0.87
	C/P	1.28	2.10
	C/SPT/P	1.19	2.28
	SPT/P	2.63	13.89

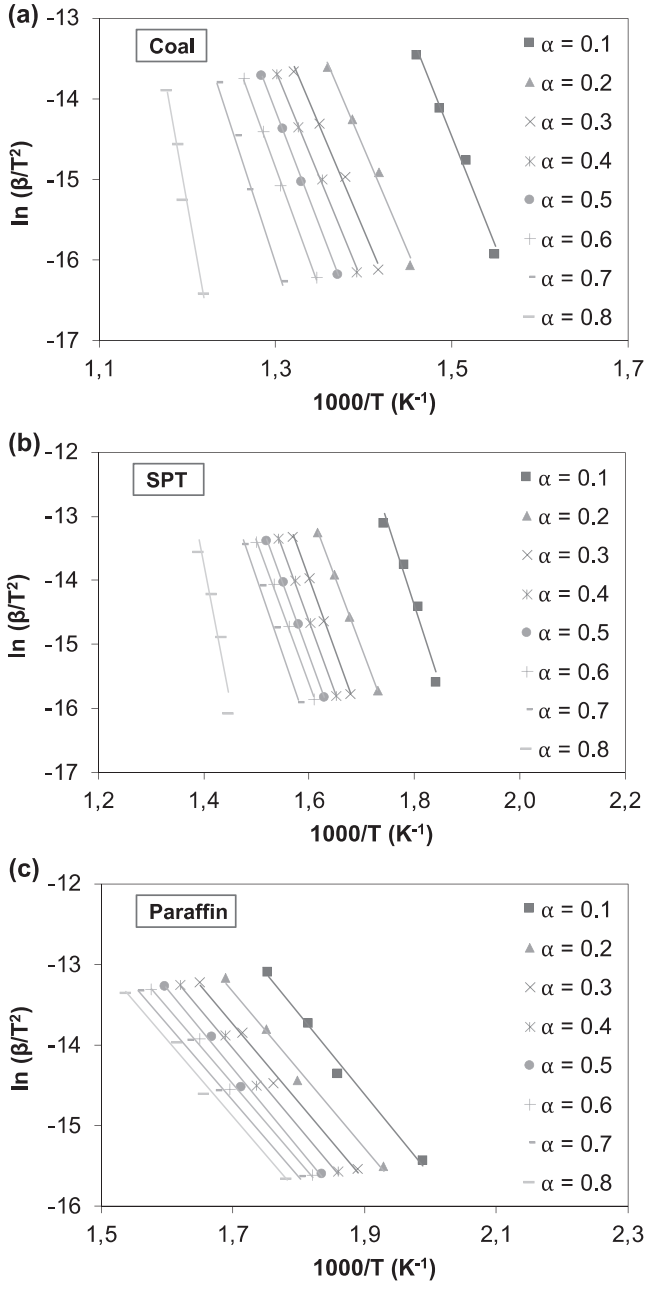

Fig. 2. Linear plots for calculation of Ea using KAS method for: (a) Coal, (b) SPT and (c) Paraffin.

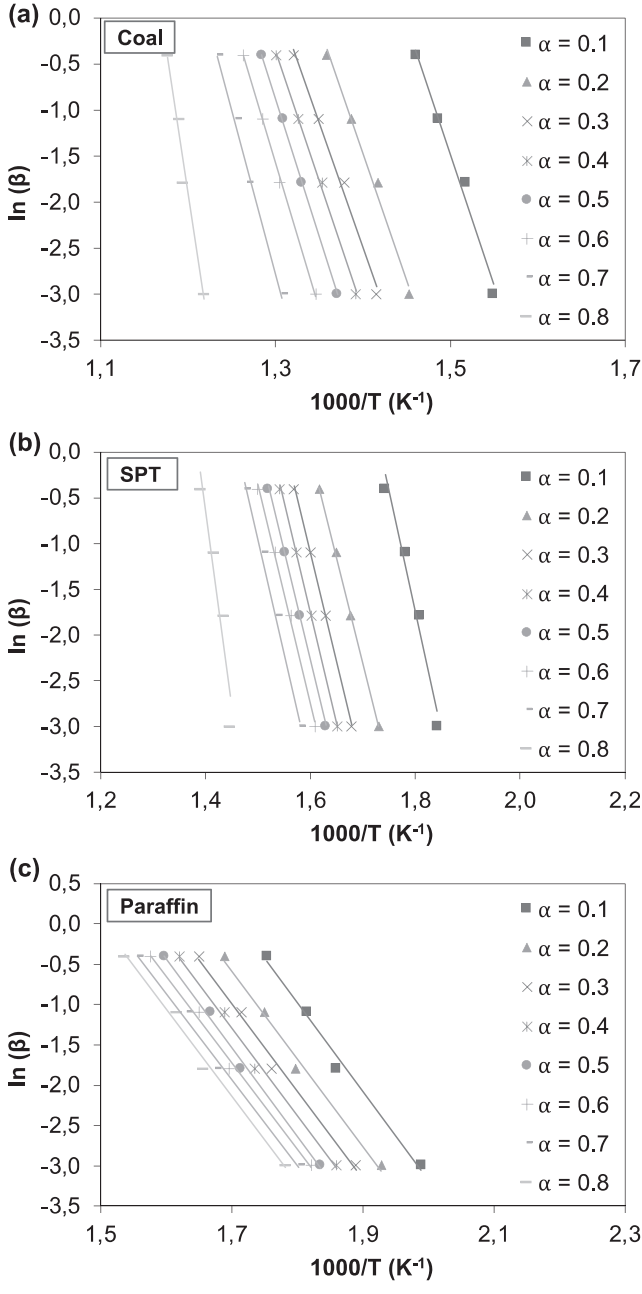

Fig. 3. Linear plots for calculation of Ea using FWO method for: (a) Coal, (b) SPT and (c) Paraffin.

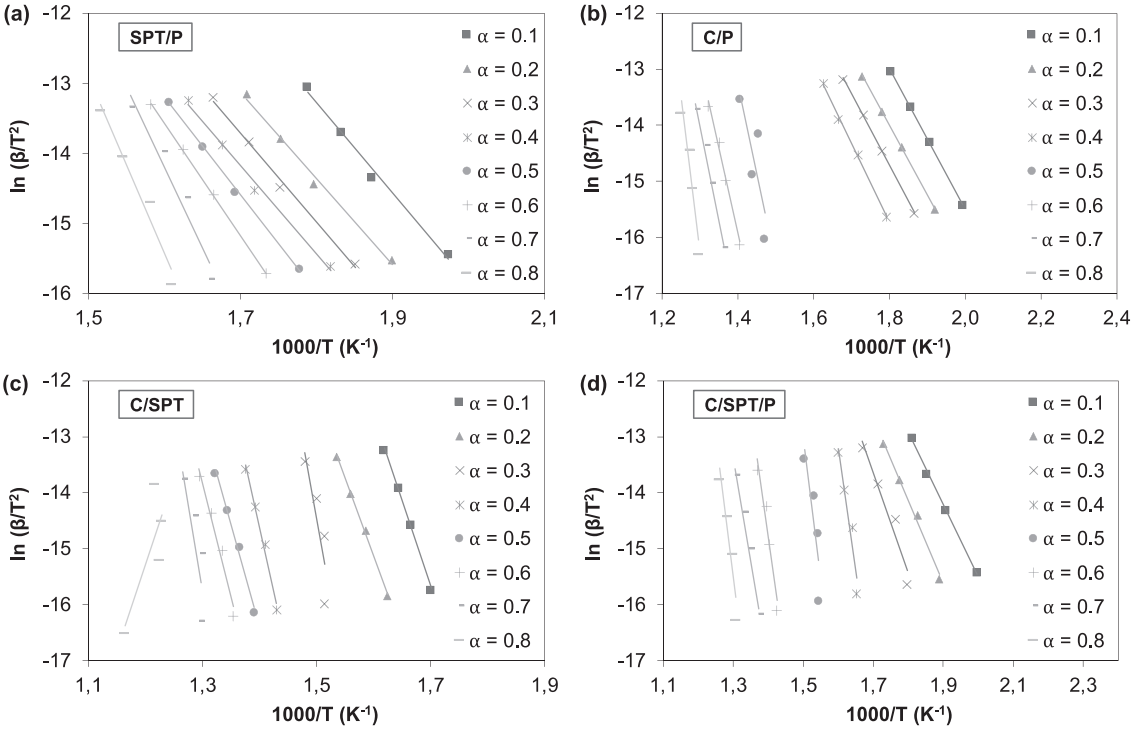

Fig. 4. Linear plots for calculation of Ea using KAS method for: (a) SPT/P, (b) C/P, (c) C/SPT and (d) C/SPT/P.

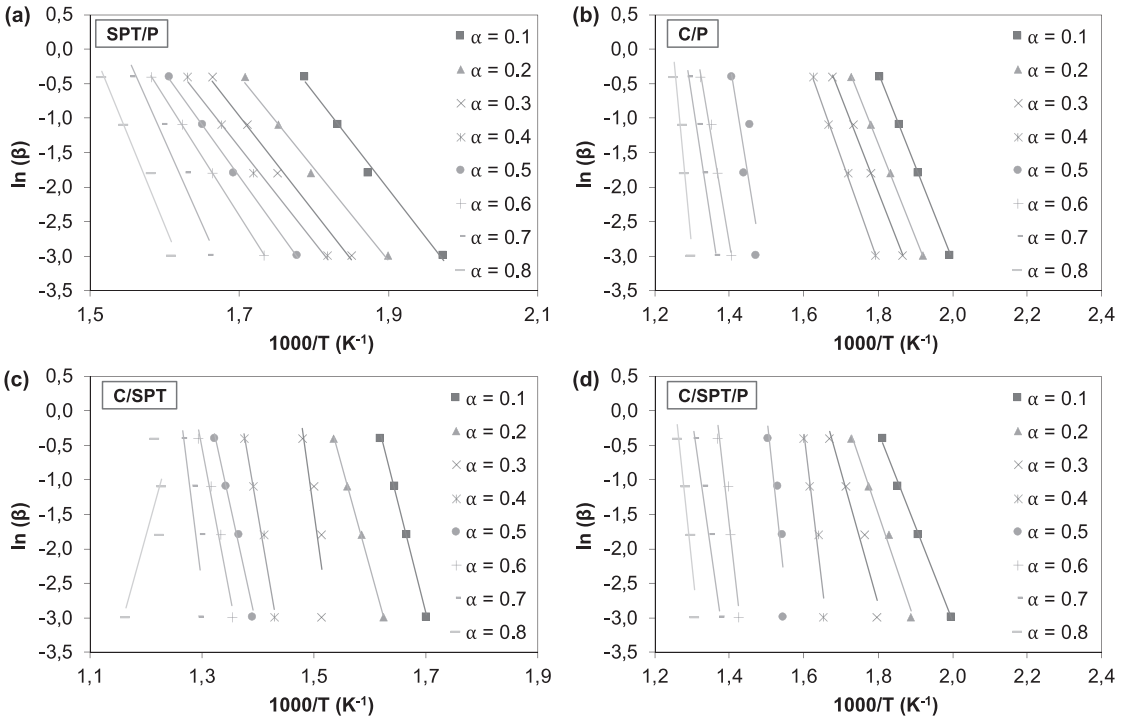

Fig. 5. Linear plots for calculation of Ea using FWO method for: (a) SPT/P, (b) C/P, (c) C/SPT and (d) C/SPT/P.

level of conversion calculated from these linear plots are detailed at Tables 2 and 3. Also, the frequency factor (A) values calculated with the Kissinger method from the Ea values are shown in Tables 2 and 3. Thermodynamic parameters corresponding to the pyrolysis of individual components and their blends, using the apparent activation energy obtained from the Friedman method at a heating rate of 3°C/min, are presented at Tables 4 and 5, respectively. Finally, Fig. 6 shows theoretical and experimental plots for prediction of solid state reaction mechanism using Criado method (Z-master plot) of paraffin for different initial weights (1.8, 5 and 10 mg).

Various files containing raw data obtained in a thermobalance from the thermal decomposition of the samples studied, using different heating rates and initial masses have been uploaded to Mendeley Data. Kinetic and thermodynamic parameters were obtained by applying isoconversional methods and Eyring equations.

2. Experimental Design, Materials and Methods

Pine sawdust (Volatile matter = 79.4 wt% db and Ash = 0.3 wt% db) was obtained as waste from the timber industry and was torrefied at 300°C in a rotary oven. The paraffin is a commercial product from Sigma Aldrich (VWW, CAS: 64742-51-4) and C is a bituminous coal (Volatile matter = 31.5 wt% db and Ash = 7.3 wt% db) normally used by the steel industry. The pyrolysis experiments were carried out in a TA Instruments SDT 2960 thermoanalyzer. Samples of around 10 mg with a particle size of <0.212 mm were used for each pyrolysis experiment. The samples were pyrolyzed from room temperature to 1000 °C, at 3, 10, 20, and 40 °C/min. Nitrogen with a purity higher than 99.9997% was used to maintain an inert atmosphere at a flow rate of 100 mL/min, α-alúmina was used as reference material in all tests. The thermobalance was calibrated using sample masses of 295.249 and 288.909 mg. The temperature was calibrated using the fusion temperature of Zn and Ag metals. In order to ensure repeatability, each experiment was repeated at least twice. The derivative of the weight loss curve (DTG curve) was calculated from the data obtained from thermogravimetric analysis (TG) as in Eq. (1):

$$DTG = \frac{1}{m_i} \cdot \frac{m_{ti+1} - m_{ti}}{t_{i+1} - t_i} \tag{1}$$

The experimental mass loss and DTG curves were compared to the calculated profile by applying the additivity law, taking into account the composition of the blends as in Eq. (2):

$$Y_{cal} = f_1 \cdot Y_1 + f_2 \cdot Y_2 \tag{2}$$

where, f_1, f_2, and f_3 are the fractions of components 1 and 2 in the mixture, and Y_1 and Y_2, are the mass loss or the derivative of the mass loss with time (dm/dt) for components 1 and 2, respectively.

The standard deviation associated to thermogravimetric analysis in the case of heating rate 3 °C/min was 0.005% for maximum DTG, 1.01 °C for Tmax and 0.42% for residue at 1000°C.

1. Descriptions and formulations of iso-conversional, Criado methods and thermodynamic study

The general kinetic model that describes the degradation process during non-isothermal pyrolysis is expressed by Eq. (3):

$$\frac{d\alpha}{dt} = k(T) \cdot f(\alpha) \tag{3}$$

where α is the conversion, t is time, f(α) is a function that represents the reaction model and will depend on the reaction mechanism and k(T) is the reaction constant that depends on the temperature. Considering that the rate constant is a function of temperature and can be expressed by the Arrhenius law, Eq. (3) can be transformed into

$$\frac{d\alpha}{dt} = Ae^{\frac{-E_a}{RT}} f(\alpha) \tag{4}$$

Table 2
The activation energy of coal, SPT and paraffin at different level of conversion using Friedman, KAS and FWO methods.

		Friedman method			KAS method			FWO method		
Conversion	Tp (°C)	Ea (kJ/mol)	R^2	A (s^{-1})	Ea (kJ/mol)	R^2	A (s^{-1})	Ea (kJ/mol)	R^2	A (s^{-1})
Coal										
0.1	445.12	216.41	0.9874	1.38E+13	227.62	0.9858	9.50E+13	216.41	0.9872	1.38E+13
0.2	445.12	205.70	0.9873	2.19E+12	214.87	0.9896	1.06E+13	205.70	0.9907	2.19E+12
0.3	445.12	215.76	0.9979	1.24E+13	213.28	0.9915	8.06E+12	215.76	0.9925	1.24E+13
0.4	445.12	250.78	0.9948	5.05E+15	222.68	0.9982	4.06E+13	250.78	0.9984	5.05E+15
0.5	445.12	269.56	0.9887	1.26E+17	236.95	0.9995	4.71E+14	269.56	0.9996	1.26E+17
0.6	445.12	265.91	0.9968	6.75E+16	249.35	0.9983	3.95E+15	265.91	0.9985	6.75E+16
0.7	445.12	326.70	0.9879	2.19E+21	281.71	0.9921	1.01E+18	326.70	0.9928	2.19E+21
0.80	445.12	569.58	0.9755	1.76E+39	505.81	0.9721	3.59E+34	569.58	0.9736	1.76E+39
Average[a]		290.05			269.03			290.05		
SPT										
0.1	348.33	199.99	0.9784	2.01E+14	208.31	0.9694	1.05E+15	206.83	0.9720	7.81E+14
0.2	348.33	189.33	0.9994	2.41E+13	190.47	0.9997	3.03E+13	181.06	0.9997	4.66E+12
0.3	348.33	190.50	0.9990	3.05E+13	187.94	0.9991	1.83E+13	188.38	0.9992	2.00E+13
0.4	348.33	184.42	0.9987	9.10E+12	187.50	0.9988	1.68E+13	188.12	0.9989	1.90E+13
0.5	348.33	185.70	0.9974	1.17E+13	186.87	0.9990	1.48E+13	187.67	0.9992	1.74E+13
0.6	348.33	198.87	0.9914	1.61E+14	187.76	0.9967	1.77E+13	188.65	0.9971	2.11E+13
0.7	404.50	213.61	0.9830	8.18E+13	229.83	0.9622	1.57E+15	228.88	0.9656	1.32E+15
0.8	404.50	264.35	0.9896	8.25E+17	252.07	0.9918	8.90E+16	250.81	0.9925	7.08E+16
Average[a]		203.35			203.84			202.55		
Paraffin (1.8 mg)										
0.1	255.01	81.49	0.9847	1.76E+08	82.77	0.9896	1.46E+08	87.27	0.9909	2.71E+08
0.2	255.01	80.48	0.9896	5.09E+08	80.85	0.9894	2.48E+08	85.61	0.9911	4.77E+08
0.3	255.01	80.80	0.9943	3.14E+08	80.80	0.9916	3.19E+08	85.74	0.9928	6.30E+08
0.4	255.01	80.63	0.9907	4.33E+08	81.19	0.9936	3.54E+08	86.21	0.9944	7.21E+08
0.5	255.01	79.79	0.9865	7.23E+08	81.79	0.9937	4.31E+08	86.21	0.9944	8.90E+08
0.6	255.01	78.59	0.9836	1.40E+09	79.34	0.9933	5.09E+08	84.67	0.9940	1.07E+09
0.7	255.01	79.10	0.9739	4.03E+09	79.11	0.9912	7.90E+08	84.58	0.9924	1.66E+09
0.8	255.01	80.87	0.9771	1.14E+10	79.49	0.9885	1.08E+09	85.04	0.9901	2.31E+09
Average[a]		80.22			80.67			85.67		
Paraffin (5 mg)										
0.1	260.12	216.41	0.9874	4.04E+04	227.62	0.9858	2.30E+06	216.41	0.9872	5.44E+06
0.2	260.12	205.70	0.9873	2.35E+04	214.87	0.9896	1.96E+05	205.70	0.9907	5.57E+05
0.3	260.12	215.76	0.9979	3.64E+04	213.28	0.9915	9.97E+04	215.76	0.9925	3.05E+05
0.4	260.12	250.78	0.9948	9.63E+03	222.68	0.9982	6.36E+04	250.78	0.9984	2.05E+05
0.5	260.12	269.56	0.9887	7.51E+04	236.95	0.9995	5.84E+04	269.56	0.9996	1.94E+05
0.6	260.12	265.91	0.9968	4.41E+04	249.35	0.9983	4.93E+04	265.91	0.9985	1.69E+05
0.7	260.12	326.70	0.9879	9.20E+04	281.71	0.9921	4.61E+04	326.70	0.9928	1.62E+05
0.80	260.12	569.58	0.9755	3.74E+05	505.81	0.9721	5.47E+04	569.58	0.9736	1.96E+05
Average[a]		290.05			269.03			290.05		
Paraffin (10 mg)										
0.1	280.43	81.49	0.9847	7.82E+04	82.77	0.9896	1.05E+05	87.27	0.9909	2.94E+05
0.2	280.43	80.48	0.9896	6.21E+04	80.85	0.9894	6.76E+04	85.61	0.9911	2.01E+05
0.3	280.43	80.80	0.9943	6.68E+04	80.80	0.9916	6.68E+04	85.74	0.9928	2.07E+05
0.4	280.43	80.63	0.9907	6.42E+04	81.19	0.9936	7.30E+04	86.21	0.9944	2.31E+05
0.5	280.43	79.79	0.9865	5.29E+04	81.79	0.9937	8.38E+04	86.21	0.9944	2.31E+05
0.6	280.43	78.59	0.9836	4.02E+04	79.34	0.9933	4.78E+04	84.67	0.9940	1.62E+05
0.7	280.43	79.10	0.9739	4.51E+04	79.11	0.9912	4.52E+04	84.58	0.9924	1.59E+05
0.8	280.43	80.87	0.9771	6.78E+04	79.49	0.9885	4.94E+04	85.04	0.9901	1.76E+05
Average[a]		80.22			80.67			85.67		

[a] Only values with $R^2 > 0.9$ were considered to calculate the average value.

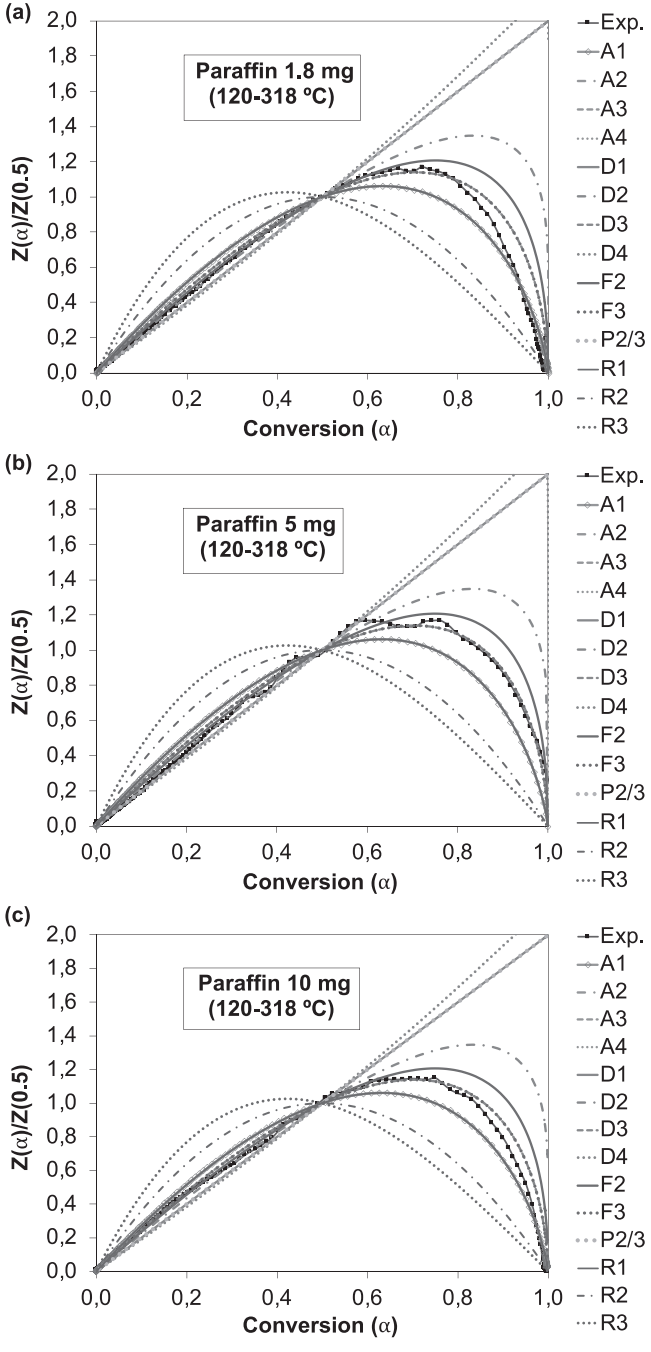

Fig. 6. Theoretical and experimental plots for prediction of solid state reaction mechanism using Criado method (Z-master plot) of: (a) paraffin (1.8 mg), (b) paraffin (5 mg) and (c) paraffin (10 mg).

Table 3
The activation energy of blends at different level of conversion using Friedman, KAS and FWO methods.

		Friedman method			KAS method			FWO method		
Conversion	Tp (°C)	Ea (kJ/mol)	R^2	A (s^{-1})	Ea (kJ/mol)	R^2	A (s^{-1})	Ea (kJ/mol)	R^2	A (s^{-1})
C/SPT										
0.1	342.21	251.96	0.9955	9.79E+18	253.22	0.9968	1.26E+19	250.41	0.9972	7.18E+18
0.2	342.21	230.90	0.9976	1.46E+17	230.95	0.9987	1.48E+17	229.69	0.9988	1.15E+17
0.3	450.02	650.13	0.8354	6.83E+44	486.02	0.7479	7.14E+32	473.72	0.7575	9.01E+31
0.4	450.02	317.79	0.9882	3.29E+20	376.60	0.9836	6.91E+24	369.89	0.9849	2.22E+24
0.5	450.02	289.90	0.9843	2.91E+18	298.58	0.9861	1.27E+19	295.79	0.9874	7.89E+18
0.6	450.02	321.19	0.9894	5.86E+20	341.56	0.9719	1.85E+22	336.77	0.9740	8.20E+21
0.7	450.02	415.62[a]	0.9801	5.02E+27	349.27[a]	0.9854	6.80E+22	345.39[a]	0.9868	3.53E+22
0.8	450.02	817.59[a]	0.4298	1.07E+57	618.16[a]	0.4526	3.19E+42	605.02[a]	0.4661	3.50E+41
Average [b]		304.56			308.36			304.66		
C/P										
0.1	257.23	102.37	0.9995	2.65E+07	104.51	0.9995	4.38E+07	107.66	0.9996	9.24E+07
0.2	257.23	104.54	0.9992	4.42E+07	103.18	0.9998	3.20E+07	106.74	0.9999	7.43E+07
0.3	257.23	115.06	0.9974	5.28E+08	106.05	0.9990	6.32E+07	109.76	0.9992	1.52E+08
0.4	257.23	157.82	0.9993	1.18E+13	117.63	0.9978	9.67E+08	121.06	0.9981	2.17E+09
0.5	450.00	242.37	0.8289	8.97E+14	263.14	0.6771	3.08E+16	261.12	0.6956	2.19E+16
0.6	450.00	255.66	0.9988	8.63E+15	251.47	0.9846	4.22E+15	250.63	0.9861	3.66E+15
0.7	450.00	334.70	0.9820	5.78E+21	286.05	0.9885	1.51E+18	283.83	0.9895	1.04E+18
0.8	450.00	585.95	0.8930	1.43E+40	454.86	0.9096	3.76E+30	444.78	0.9142	6.88E+29
Average [b]		236.59			203.39			203.49		
C/SPT/P										
0.1	259.33	107.52	0.9993	8.06E+07	106.02	0.9977	5.66E+07	109.08	0.9980	1.16E+08
0.2	259.33	135.46	0.9783	5.59E+10	122.58	0.9891	2.76E+09	125.26	0.9907	5.16E+09
0.3	344.00	197.70	0.9165	1.69E+14	150.52	0.9457	1.31E+10	152.21	0.9519	1.84E+10
0.4	344.00	311.79[a]	0.9756	1.21E+24	268.29[a]	0.9834	2.17E+20	264.78[a]	0.9846	1.08E+20
0.5	446.98	324.51[a]	0.8390	1.30E+21	265.27[a]	0.9426	5.37E+16	262.54[a]	0.9469	3.37E+16
0.6	446.98	311.04	0.9674	1.31E+20	378.43	0.9358	1.24E+25	371.04	0.9395	3.53E+24
0.7	446.98	322.66	0.9862	9.50E+20	303.84	0.9866	3.86E+19	300.62	0.9876	2.23E+19
0.8	446.98	507.03	0.8351	3.53E+34	415.06	0.8866	6.16E+27	406.86	0.8927	1.54E+27
Average [b]		270.46			251.25			249.05		
SPT/P										
0.1	280.00	102.28	0.9954	9.16E+06	106.97	0.9911	2.66E+07	110.07	0.9923	5.36E+07
0.2	280.00	104.53	0.9961	1.53E+07	102.66	0.9919	9.99E+06	106.34	0.9930	2.30E+07
0.3	280.00	109.72	0.9964	4.96E+07	105.85	0.9940	2.06E+07	109.60	0.9948	4.82E+07
0.4	280.00	116.36	0.9974	2.23E+08	104.80	0.9935	1.62E+07	108.77	0.9944	4.00E+07
0.5	280.00	135.73	0.9999	1.75E+10	115.71	0.9985	1.92E+08	119.32	0.9987	4.35E+08
0.6	342.29	181.05	0.9910	6.69E+12	132.60	0.9998	3.78E+08	135.58	0.9998	6.92E+08
0.7	342.29	183.31[a]	0.9991	1.05E+13	190.31	0.9504	4.29E+13	190.74	0.9554	4.68E+13
0.8	342.29	221.14	0.9456	2.06E+16	209.78	0.9598	2.13E+15	209.53	0.9635	2.02E+15
Average [b]		144.26			133.58			136.24		

[a] the value corresponding to 3°C/min was discarded for the calculation of the average. [b] The average Ea value was calculated with those with $R^2 \geq 0.9$.

Where R is the universal gas constant (8.314 J/K•mol).

If the conversion is expressed as a function of the temperature and the heating rate (ß), and integrating both sides, Eq. (4) can be transformed into Eq. (5):

$$g(\alpha) = \int_0^{\alpha} \frac{d\alpha}{f(\alpha)} = \frac{A}{\beta} \int_0^{T} e^{\frac{-Ea}{RT}}\, dT = \frac{AE_a}{\beta R} P(x) \tag{5}$$

- Friedman method. This method is the most widely used differential iso-conversional method for kinetic analysis. The Friedman equation may be derived by rearranging and taking natural

Table 4
Thermodynamic parameters for pyrolysis of individual components using the apparent activation energy obtained from the Friedman method at a heating rate of 3°C/min.

α	Stages	Tp (°C)	Ea (kJ/mol)	R^2	A (s^{-1})	$\Delta H^{\ddagger}$ (kJ/mol)	$\Delta G^{\ddagger}$ (kJ/mol)	$\Delta S^{\ddagger}$ (J/mol)
Coal								
0.1		445.12	216.41	0.9874	1.38E+13	210.43	216.89	-8.99
0.2		445.12	205.70	0.9873	2.19E+12	199.73	217.19	-24.31
0.3		445.12	215.76	0.9979	1.24E+13	209.79	216.91	-9.90
0.4	Stage I	445.12	250.78	0.9948	5.05E+15	244.80	216.01	40.09
0.5		445.12	269.56	0.9887	1.26E+17	263.58	215.58	66.84
0.6		445.12	265.91	0.9968	6.75E+16	259.93	215.66	61.64
0.7		445.12	326.70	0.9879	2.19E+21	320.73	214.43	147.99
0.8		445.12	569.58	0.9755	1.76E+39	563.61	211.11	490.77
Average[a]			290.05			284.08	215.47	95.52
SPT								
0.1	Stage I	348.33	199.99	0.9784	2.07E+14	194.83	185.67	14.74
0.2		348.33	189.33	0.9994	2.41E+13	184.16	186.11	-3.14
0.3		348.33	190.50	0.9990	3.05E+13	185.33	186.08	-1.20
0.4		348.33	184.42	0.9987	9.10E+12	179.25	186.25	-11.25
0.5		348.33	185.70	0.9974	1.17E+13	180.53	186.21	-9.13
0.6		348.33	198.87	0.9914	1.61E+14	193.70	185.86	12.63
0.7	Stage II	404.50	213.61	0.9830	8.18E+13	207.98	203.71	6.29
0.8		404.50	264.35	0.9896	8.25E+17	258.72	202.51	82.94
Average[a]			203.35			198.06	190.30	11.49
Paraffin (1.8 mg)								
0.1		255.01	109.92	0.9883	1.76E+08	105.53	158.41	-100.12
0.2		255.01	114.40	0.9648	5.09E+08	110.01	158.23	-91.30
0.3		255.01	112.36	0.9867	3.14E+08	107.97	158.31	-95.31
0.4	Stage I	255.01	113.72	0.9851	4.33E+08	109.33	158.26	-92.64
0.5		255.01	115.89	0.9889	7.23E+08	111.50	158.18	-88.38
0.6		255.01	118.68	0.9899	1.40E+09	114.29	158.07	-82.89
0.7		255.01	123.16	0.9869	4.03E+09	118.77	157.91	-74.10
0.8		255.01	127.56	0.9806	1.14E+10	123.17	157.75	-65.48
Average[a]			116.96		9.32E+08	112.57	158.14	-86.28
Paraffin (5 mg)								
0.1	Stage I	260.12	75.57	0.9785	4.04E+04	71.14	161.73	-169.87
0.2		260.12	73.31	0.9780	2.35E+04	68.88	161.86	-174.38
0.3		260.12	75.14	0.9814	3.64E+04	70.71	161.76	-170.74
0.4		260.12	69.58	0.9684	9.63E+03	65.15	162.10	-181.80
0.5		260.12	78.17	0.9891	7.51E+04	73.74	161.58	-164.73
0.6		260.12	75.94	0.9868	4.41E+04	71.50	161.71	-169.15
0.7		260.12	79.02	0.9921	9.20E+04	74.59	161.53	-163.03
0.8		260.12	84.92	0.9959	3.74E+05	80.49	161.21	-151.38
Average[a]			76.46		4.99E+04	72.02	161.68	-168.14
Paraffin (10 mg)								
0.1		280.43	81.49	0.9847	1.09E+05	76.96	165.03	-161.79
0.2		280.43	80.48	0.9896	8.63E+04	75.96	165.09	-163.74
0.3		280.43	80.80	0.9943	9.30E+04	76.28	165.07	-163.12
0.4	Stage I	280.43	80.63	0.9907	8.92E+04	76.10	165.08	-163.46
0.5		280.43	79.79	0.9865	7.34E+04	75.26	165.13	-165.09
0.6		280.43	78.59	0.9836	5.54E+04	74.06	165.20	-167.42
0.7		280.43	79.10	0.9739	6.24E+04	74.57	165.17	-166.43
0.8		280.43	80.87	0.9771	9.44E+04	76.34	165.07	-162.99
Average[a]			80.22			75.69	165.11	-164.25

[a] The average Ea value was calculated with those with $R^2 \geq 0.9$.

Table 5
Thermodynamic parameters for pyrolysis of blends using the apparent activation energy obtained from the Friedman method at a heating rate of 3°C/min.

α	Stages	Tp (°C)	Ea (kJ/mol)	R^2	A (s^{-1})	$\Delta H^{\ddagger}$ (kJ/mol)	$\Delta G^{\ddagger}$ (kJ/mol)	$\Delta S^{\ddagger}$ (J/mol)
SPT/P								
0.1		280.00	102.28	0.9954	9.16E+06	97.68	166.87	-125.09
0.2	Stage I	280.00	104.53	0.9961	1.53E+07	99.93	166.77	-120.83
0.3		280.00	109.72	0.9964	4.96E+07	105.12	166.55	-111.05
0.4		280.00	116.36	0.9974	2.23E+08	111.76	166.28	-98.55
0.5		280.00	135.73	0.9999	1.75E+10	131.14	165.57	-62.25
0.6		342.29	181.05	0.9910	6.69E+12	175.93	184.38	-13.73
0.7	Stage II	342.29	183.31	0.9991	1.05E+13	178.19	184.32	-9.95
0.8		342.29	221.14	0.9456	2.06E+16	216.02	183.36	53.07
Average[a]			144.26			139.47	173.01	-61.05
C/P								
0.1		257.23	102.37	0.9995	2.65E+07	97.96	159.44	-115.92
0.2	Stage I	257.23	104.54	0.9992	4.42E+07	100.13	159.35	-111.66
0.3		257.23	115.06	0.9974	5.28E+08	110.65	158.93	-91.03
0.4		257.23	157.82	0.9993	1.18E+13	153.42	157.53	-7.77
0.5		450.00	242.37	0.8289	8.97E+14	236.36	217.80	25.66
0.6	Stage II	450.00	255.66	0.9988	8.63E+15	249.65	217.48	44.48
0.7		450.00	334.70	0.9820	5.78E+21	328.68	215.86	156.01
0.8		450.00	585.95	0.8930	1.43E+40	579.93	212.50	508.11
Average[a]			236.59			231.49	183.01	54.60
C/SPT								
0.1	Stage I	342.21	251.96	0.9955	9.79E+18	246.85	182.66	104.31
0.2		342.21	230.90	0.9976	1.46E+17	225.79	183.11	69.36
0.3		450.02	650.13	0.8354	6.83E+44	644.12	211.88	597.70
0.4		450.02	317.79	0.9882	3.29E+20	311.77	216.18	132.18
0.5	Stage II	450.02	289.90	0.9843	2.91E+18	283.89	216.73	92.86
0.6		450.02	321.19	0.9894	5.86E+20	315.18	216.12	136.99
0.7		450.02	415.62	0.9801	5.02E+27	409.60	214.57	269.70
0.8		450.02	817.59	0.4298	1.07E+57	811.58	210.50	831.17
Average[a]			304.56			298.85	204.90	134.23
C/SPT/P								
0.1	Stage I	259.33	107.52	0.9993	8.06E+07	103.10	159.91	-106.69
0.2		259.33	135.46	0.9783	5.59E+10	131.03	158.89	-52.31
0.3	Stage II	344.00	197.70	0.9165	1.69E+14	192.57	184.48	13.10
0.4		344.00	311.79	0.9756	1.21E+24	306.66	182.15	201.76
0.5		446.98	324.51	0.8390	1.30E+21	318.52	215.07	143.66
0.6	Stage III	446.98	311,04	0.9674	1.31E+20	305.05	215.33	124.59
0.7		446.98	322.66	0.9862	9.50E+20	316.67	215.11	141.04
0.8		446.98	507.03	0.8351	3.53E+34	501.04	212.40	400.82
Average[a]			270.46			265.16	189.75	103.19

[a] The average Ea value was calculated with those with $R^2 \geq 0.9$.

logarithms on both sides of Eq. (5):

$$\ln\left(\beta\frac{d\alpha}{dt}\right) = \ln[A\ f(\alpha)] - \frac{E\alpha}{RT} \tag{6}$$

Where Eα and Tα are the activation energy and temperature at conversion α, respectively. The Eα can be calculated from the slope of the plot of the left hand side of Eq. (6) versus the inverse of the temperature, at constant values of α.

- Kissinger-Akahira-Sunose (KAS) method. The KAS equation is derived from Eq. (5) and Murray and White's approximation, $p(x) = e^x/x^2$ for the temperature integral.

$$ln\left(\frac{\beta}{T_\alpha^2}\right) = ln\left(\frac{AE_\alpha}{Rg(x)}\right) - \frac{E_\alpha}{RT_\alpha} \tag{7}$$

  The plot between ln $(\beta/T^2{}_\alpha)$ and $1/T_\alpha$, at a constant value of conversion gives a straight line, whose slope can be used to calculate activation energy.
- Flynn-Wall-Ozawa (FWO) method. The FWO equation is also derived from Eq. (5). In this method Doyle's approximation [6]: $p(x) = \exp(-2.315+0{:}4567x)$, is used for the temperature integral, where $x = Ea/RT$. The FWO equation can be written in the following form Eq. (8):

$$\ln\beta = \ln\left(\frac{AE_\alpha}{Rg(\alpha)}\right) - 5.3305 - 1.052\frac{E_\alpha}{RT_\alpha} \tag{8}$$

The slope obtained by plotting $\ln(\beta)$ *vs* $1/T_\alpha$ can be used to compute activation energy. Compared to the differential method (Friedman), the integral methods involve an intrinsic error in calculation of activation energy due to the temperature integral.

Prediction of reaction model

The kinetic mechanism of solid state reaction was investigated using two methodologies: The Criado method and the Coats-Redfern method.

- The Criado method uses the Z-master plot shown in Eq. (9).

$$\frac{Z(\alpha)}{Z(0.5)} = \frac{f(\alpha)\cdot g(\alpha)}{f(\alpha)\cdot g(0.5)} = \left(\frac{T_\alpha}{T_{0.5}}\right)^2 \cdot \frac{(d\alpha/dt)_\alpha}{(d\alpha/dt)_{0.5}} \tag{9}$$

  Master plots are plots which depend on the reaction kinetic model however they are independent of kinetic parameters like activation energy and frequency factor. Eq. (9) is used to generate the master plots corresponding to different reaction mechanisms.

Thermodynamic study

Once the activation energy and frequency factor were determined at different levels of conversion, the thermodynamic parameters, such as change of enthalpy ($\Delta H^\ddagger$), Gibbs free energy ($\Delta G^\ddagger$), and entropy ($\Delta S^\ddagger$) of the transition states were calculated using the Eyring equations (Eqs 10–12):

$$\Delta H^\ddagger = E_\alpha - RT_\alpha \tag{10}$$

$$\Delta G^\ddagger = E_\alpha + RT_p\, ln\left(\frac{K_B\cdot T_p}{hA}\right) \tag{11}$$

$$\Delta S^\ddagger = \frac{\Delta H^\ddagger - \Delta G^\ddagger}{T_p} \tag{12}$$

Where, K_B is the Boltzman constant (1.381×10^{-23} J/K) and h is the Plank constant (6.626×10^{-34} J/s).

Ethics Statement

The authors declare that this work has been done according to the ethical requirements for publication in Data in Brief.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

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