

## Assessing the life cycle environmental impacts of titania nanoparticle production by continuous flow hydrothermal synthesis

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### Life Cycle Assessment

#### Precursors

#### Titanium Oxysulphate (TiOS)

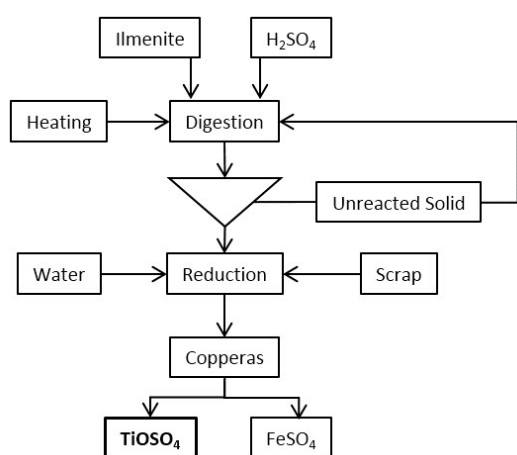


Table 1. Material and energy inputs required for the production of 1 kg of a 15% TiOS solution.

Inputs	
Ilmenite (55%TiO <sub>2</sub> )	0.14 kg
Sulfuric acid (95%)	0.30 kg
Iron	0.01 kg
Water	0.83 kg
Natural Gas	0.05 MJ
Electric Cooling	0.02 MJ

Figure 1. Scheme for the production of TiOS, which includes the steps of digestion reduction and separation of products.

#### Titanium tetrachloride (TiCl<sub>4</sub>)

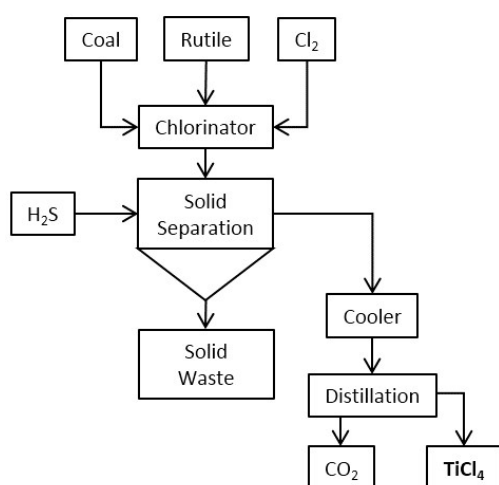


Table 2. Material and energy inputs required to produce 1 kg of TiCl<sub>4</sub>.

Inputs	
Coal	0.10 kg
Chlorine	0.75 kg
Rutile	0.43 kg
Hydrogen Sulphide	Trace
CO <sub>2</sub> emission	0.27
Electric Cooling	0.03 MJ

Figure 2. Scheme for the production of TiCl<sub>4</sub>, including the chlorination process and the stages of separation.

### Titanium isopropoxide (TiPO)

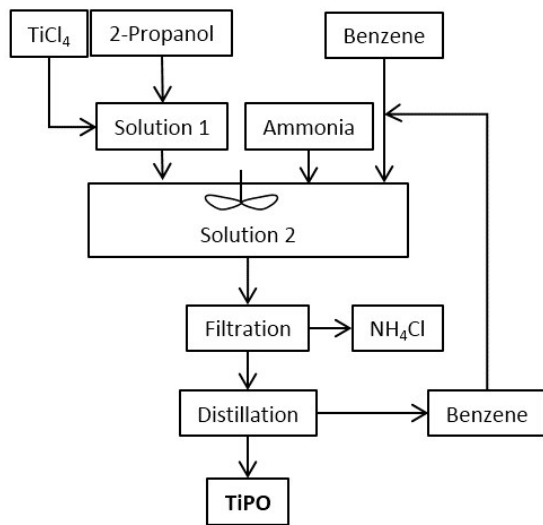


Table 3. Material and energy inputs required to produce 1 kg of TiPO.

Inputs	
TiCl <sub>4</sub>	0.83 kg
2-Propanol	1.05 kg
Ammonia	0.30 kg
Benzene	1.60 kg
Natural Gas	1.19 MJ
Electricity	0.03 MJ

Figure 3. Scheme for the production of TiPO according to the literature with the stages of mixing and separation.

### Titanium bis(ammonium lactate) dihydroxide (TiBALD)

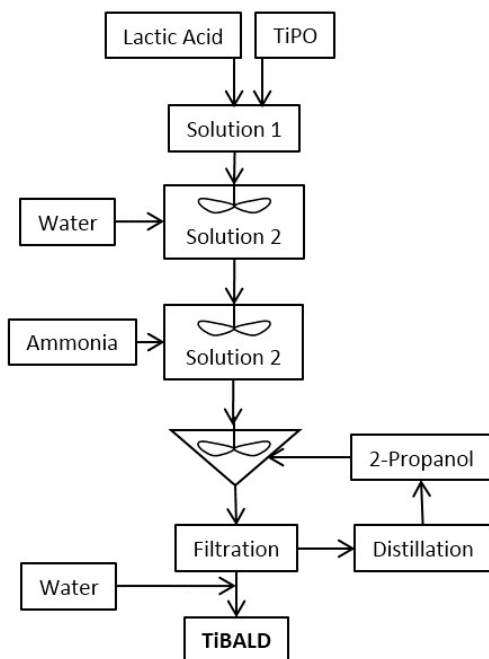


Table 4. . Material and energy inputs required to produce 1 kg of TiBALD.

Inputs	
TiPO	0.63 kg
Lactic Acid	0.40 kg
Water	3.78 kg
Ammonia (28%)	0.26 kg
2-Propanol	0.30 MJ
Natural Gas	9.18 MJ
Electric Stirring	0.15 MJ

Figure 4. Scheme for the production of TiBALD, which includes the inlets of lactic acid and ammonia, the precipitation with 2-propanol and the separation stages.

Potassium titanium oxide oxalate dihydroxide (PTOOD)

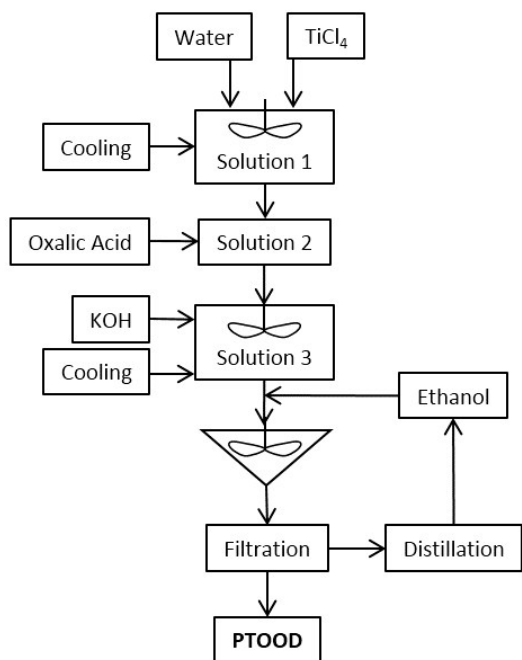


Table 5. Material and energy inputs required to produce 1 kg of PTOOD

Inputs	
TiCl <sub>4</sub>	0.54 kg
Water	8.47 kg
Oxalic Acid	0.51 kg
KOH	0.33 kg
Ethanol	0.01 kg
Natural Gas	21.96 MJ
Electric Stirring	0.04 MJ
Electric Cooling	0.74 MJ

Figure 5. Scheme for the production of PTOOD, which includes all production and separation stages.

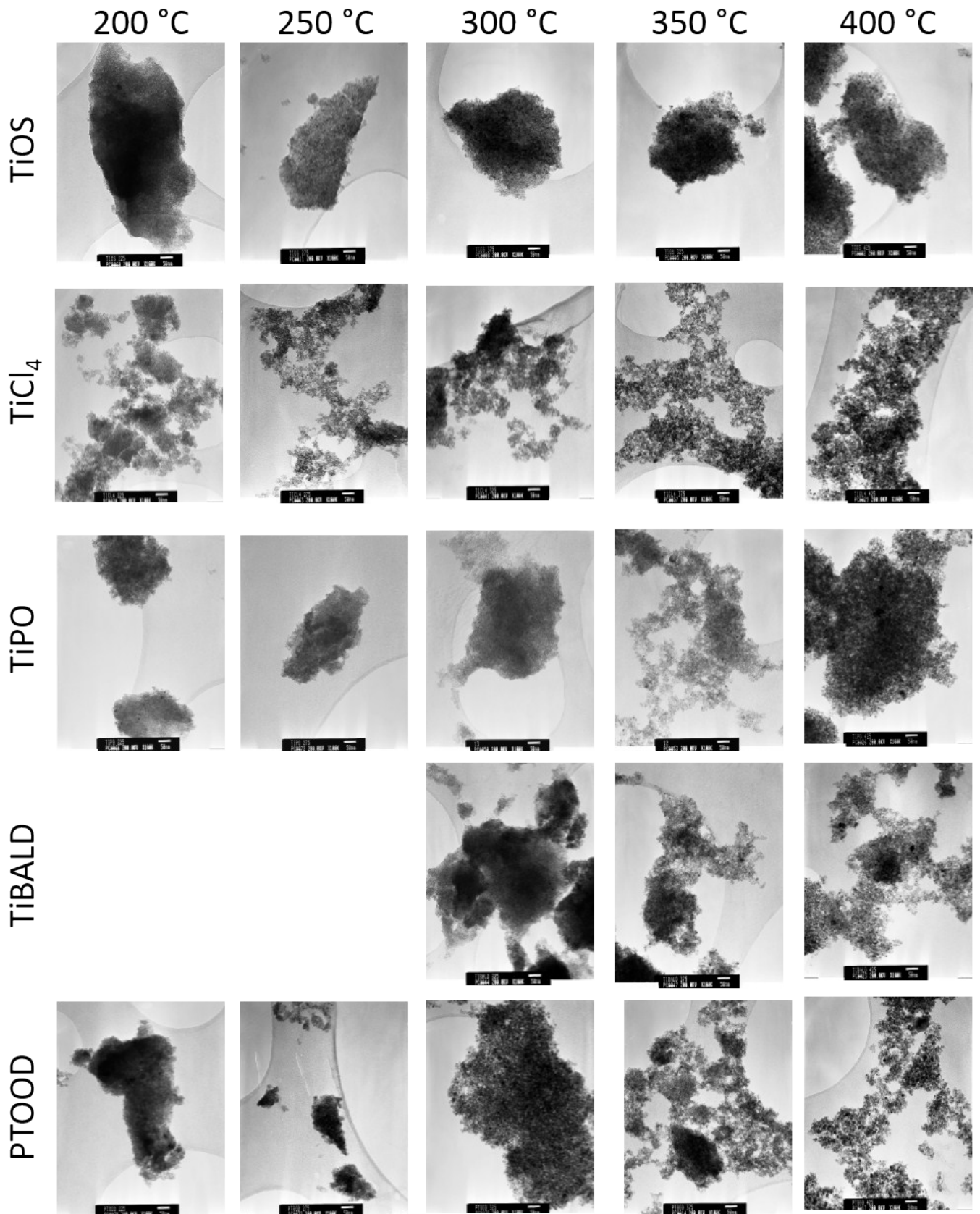


Figure 6. Representative TEM images of all samples acquired

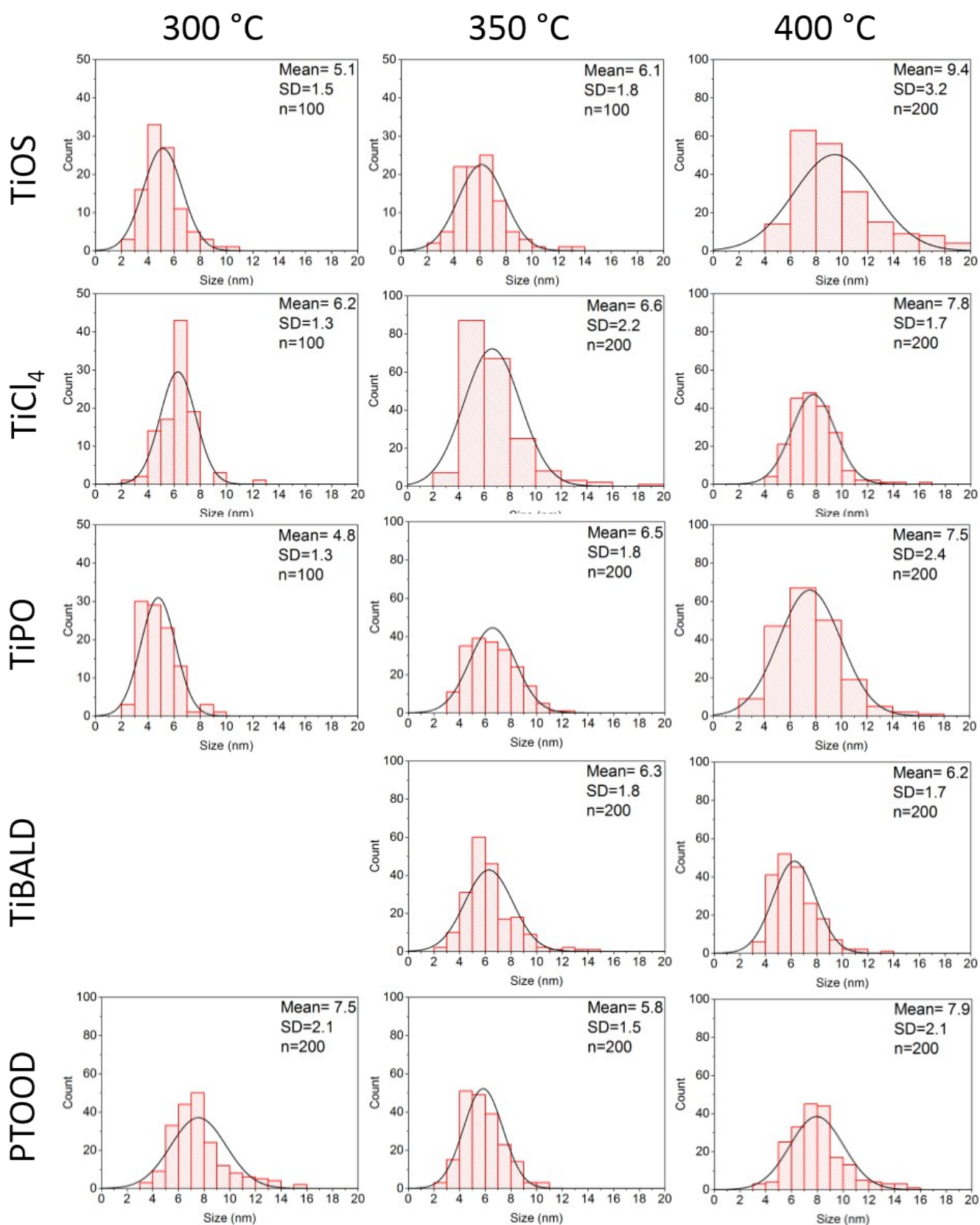


Figure 7. Size distribution histograms of all samples where possible.

Table 1. Cumulative energy demand values in MJ/kg TiO<sub>2</sub> for all of the precursors and temperatures at industrial-scale production. Temp. = Temperature, Pre. = Precursor, IPA = Isopropanol, IPA dis. = Isopropanol distillation, H<sub>2</sub>O<sub>2</sub> = Hydrogen Peroxide, Pack. = Packaging, Trans. = Transport, DIW = Deionised Water, Elec. = Electricity, H&C = Heating and Cooling, CP = Cleaning process, PP = Postprocessing, Wash = Washing, Neu. = Neutralization and WWT = Water waste treatment.

Precursor	Temp. (°C)	Pre.	IPA	IPA dis.	H <sub>2</sub> O <sub>2</sub>	Pack.	Trans.	DIW	Elec.	H&C	CP	PP	Wash	Neu.	WWT
TiOS	200	26.7	-	-	-	4.7E-02	10.8	2.7	15.4	46.5	2.2E-02	0.2	0.7	16.2	13.7
	250	18.4	-	-	-	3.2E-02	7.5	1.9	10.6	42.6	1.1E-02	0.1	0.5	11.2	9.5
	300	18.4	-	-	-	3.2E-02	7.5	1.9	10.6	52.3	1.1E-02	0.1	0.5	11.2	9.5
	350	18.8	-	-	-	3.3E-02	7.6	1.9	10.8	75.8	1.1E-02	0.1	0.5	11.4	9.7
	400	18.4	-	-	-	3.2E-02	7.5	1.9	10.6	89.3	1.1E-02	0.1	0.5	11.2	9.3
TiCl <sub>4</sub>	200	171.3	7.5	164.1	-	3.0E-02	3.0	3.2	23.6	71.3	3.3E-02	61.7	1.1	225.2	22.7
	250	140.2	6.1	134.3	-	2.5E-02	2.5	2.6	19.3	77.4	2.2E-02	33.7	0.9	122.8	16.5
	300	137.6	6.0	131.9	-	2.4E-02	2.4	2.6	19.0	93.3	2.2E-02	33.1	0.9	120.6	16.2
	350	115.1	5.0	110.3	-	2.0E-02	2.0	2.1	15.9	110.9	2.2E-02	20.8	0.7	75.6	12.6
	400	100.1	4.4	95.9	-	1.8E-02	1.8	1.9	13.8	115.9	2.2E-02	18.1	0.6	65.8	11.0
TiPO	200	945.0	3.9	83.1	-	1.6E-02	2.3	1.6	14.0	36.9	1.1E-02	0.1	0.5	-	7.8
	250	839.1	3.4	73.8	-	1.4E-02	2.3	1.5	12.4	43.4	1.1E-02	0.1	0.5	-	7.0
	300	847.6	3.5	74.6	-	1.4E-02	2.1	1.5	12.5	53.9	1.1E-02	0.1	0.5	-	7.0
	350	884.1	3.6	77.8	-	1.5E-02	2.2	1.5	13.1	79.9	1.1E-02	15.0	0.5	54.3	9.2
	400	1227.3	5.0	108.0	-	2.0E-02	3.0	2.1	18.2	133.2	2.2E-02	20.8	0.7	76.7	12.8
TiBALD	200	5547.1	-	-	124.5	0.8E-02	18.3	6.3	35.7	107.0	4.4E-02	61.8	1.6	225.2	39.0
	250	2971.1	-	-	66.7	4.3E-02	9.8	3.4	19.1	76.0	2.2E-02	24.9	0.9	90.5	19.9
	300	2311.2	-	-	51.9	3.3E-02	7.6	2.6	14.9	72.6	2.2E-02	19.3	0.7	70.4	15.7
	350	2218.6	-	-	49.8	3.2E-02	7.3	2.5	14.3	99.1	2.2E-02	0.1	0.6	-	12.5
	400	1789.3	-	-	40.1	2.6E-02	5.9	2.0	11.5	96.0	1.1E-02	0.1	0.5	-	10.0
PTOOD	200	507.1	-	-	67.9	7.2E-03	6.7	3.8	20.9	58.3	2.2E-02	25.3	0.9	92.1	20.8
	250	435.8	-	-	59.3	3.1E-02	5.8	3.2	16.7	66.5	2.2E-02	21.8	0.7	79.2	17.9
	300	357.7	-	-	47.9	2.5E-02	4.7	2.7	13.7	67.0	2.2E-02	17.9	0.6	65.0	14.7
	350	336.1	-	-	45.0	2.4E-02	4.5	2.5	12.9	89.5	2.2E-02	0.1	0.6	-	11.7
	400	317.0	-	-	42.4	1.6E-02	4.2	2.4	12.2	101.4	1.1E-02	0.1	0.5	-	11.0

Table 2. Global warming potential values in kg CO<sub>2</sub>-eq/kg TiO<sub>2</sub> for all of the precursors and temperatures at industrial-scale production. Temp. = Temperature, Pre. = Precursor, IPA = Isopropanol, IPA dis. = Isopropanol distillation, H<sub>2</sub>O<sub>2</sub> = Hydrogen Peroxide, Pack. = Packaging, Trans. = Transport, DIW = Deionised Water, Elec. = Electricity, H&C = Heating and Cooling, CP = Cleaning process, PP = Postprocessing, Wash = Washing, Neu. = Neutralization and WWT = Water waste treatment.

Precursor	Temp. (°C)	Pre.	IPA	IPA dis.	H <sub>2</sub> O <sub>2</sub>	Pack.	Trans.	DIW	Elec.	H&C	CP	PP	Wash	Neu.	WWT
TiOS	200	1.7	-	-	-	1.4E-02	0.7	0.1	0.9	2.7	1.2E-03	8.9E-03	3.5E-02	1.2	4.6
	250	1.2	-	-	-	9.9E-03	0.4	0.1	0.6	2.5	6.1E-04	6.1E-03	2.4E-02	0.8	3.2
	300	1.2	-	-	-	9.9E-03	0.4	0.1	0.6	3.0	6.1E-04	6.1E-03	2.4E-02	0.8	3.2
	350	1.2	-	-	-	1.0E-02	0.5	0.1	0.6	4.4	6.1E-04	6.2E-03	2.5E-02	0.8	3.2
	400	1.2	-	-	-	9.9E-03	0.4	0.1	0.6	5.2	6.1E-04	6.1E-03	2.4E-02	0.8	3.1
TiCl <sub>4</sub>	200	9.5	0.2	9.5	-	4.5E-03	0.2	0.2	1.3	4.1	1.8E-03	3.7	5.4E-02	16.4	7.6
	250	7.8	0.2	7.8	-	3.7E-03	0.1	0.1	1.1	4.5	1.2E-03	2.0	4.4E-02	8.9	5.5
	300	7.6	0.2	7.6	-	3.6E-03	0.1	0.1	1.1	5.4	1.2E-03	2.0	4.3E-02	8.8	5.4
	350	6.4	0.2	6.4	-	3.0E-03	0.1	0.1	0.9	6.4	1.2E-03	1.2	3.6E-02	5.5	4.2
	400	5.5	0.1	5.5	-	2.6E-03	0.1	0.1	0.8	6.7	1.2E-03	1.1	3.1E-02	4.8	3.7
TiPO	200	34.0	0.1	4.8	-	3.2E-03	0.1	0.1	0.8	2.1	6.1E-04	7.0E-03	2.8E-02	-	2.6
	250	30.2	0.1	4.3	-	2.9E-03	0.1	0.1	0.7	2.5	6.1E-04	6.2E-03	2.5E-02	-	2.3
	300	30.5	0.1	4.3	-	2.9E-03	0.1	0.1	0.7	3.1	6.1E-04	6.3E-03	2.5E-02	-	2.3
	350	31.8	0.1	4.5	-	3.0E-03	0.1	0.1	0.7	4.6	6.1E-04	3.9	2.6E-02	3.9	3.1
	400	44.1	0.2	6.2	-	4.2E-03	0.2	0.1	1.0	6.4	1.2E-03	5.6	3.6E-02	5.6	4.3
TiBALD	200	224.8	-	-	6.2	2.2E-02	1.2	0.3	2.0	6.2	2.4E-03	3.7	8.1E-02	16.4	13.0
	250	120.4	-	-	3.3	1.2E-02	0.6	0.2	1.1	4.4	1.2E-03	1.5	4.3E-02	6.6	6.6
	300	93.7	-	-	2.6	9.4E-03	0.5	0.1	0.8	4.2	1.2E-03	1.2	3.4E-02	5.1	5.2
	350	89.9	-	-	2.5	9.0E-03	0.5	0.1	0.8	5.7	1.2E-03	8.1E-03	3.2E-02	-	4.1
	400	72.5	-	-	2.0	7.2E-03	0.4	0.1	0.6	5.5	6.1E-04	6.6E-03	2.6E-02	-	3.3
PTOOD	200	31.1	-	-	3.4	8.5E-03	0.4	0.2	1.2	3.4	1.2E-03	1.5	4.4E-02	6.7	6.9
	250	26.7	-	-	2.9	7.3E-03	0.4	0.2	0.9	3.8	1.2E-03	1.3	3.8E-02	5.8	6.0
	300	21.9	-	-	2.4	6.0E-03	0.3	0.1	0.8	3.8	1.3E-03	1.1	3.4E-02	4.8	4.9
	350	20.6	-	-	2.3	5.6E-03	0.3	0.1	0.7	5.2	1.2E-03	7.4E-03	3.1E-02	-	3.9
	400	19.4	-	-	2.1	3.8E-03	0.3	0.1	0.7	5.9	6.1E-04	6.9E-03	2.7E-02	-	3.7