Chapter 11

Techno-economic feasibility assessment on the viability of using waste PET (trays and coloured bottles) to produce Metal-Organic Frameworks (MOFs)

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Abstract

This work reviewed the business model of waste PET-to-MOFs from technical feasibility, economic appraisal, commercial viability, and risk assessment. A process model was developed to cover the mass balance, which considered material flows, chemical build-up, and energy requirements. The balance was based on a case of 1 kg/day, and the scalability was proved at a later stage. A financial model was then developed, and the analysis of economic appraisal and commercial viability showed that investing in MOFs will generate roughly a 5% internal rate of return (IRR) on a production capacity of 10 kg daily. Given the fact that these results are positive at a small scale, it is therefore recommended that this investment should proceed. The environmental and opportunity cost that is avoided has not been considered in the financial analysis. This can further strengthen the revenue side of this production. While a return of 5% is not the most attractive, the PET waste that would be redirected to this production contributes to the South African waste management strategy and climate change objectives. In addition, since the South

African government bond of ten years yields a return of 8.52% return, this initiative is competitive with a 5% IRR.

Keywords: Techno-economic Feasibility, Trays and Coloured Bottles, Metal-organic frameworks, Viability

1. Introduction

Polyethylene terephthalate (PET), as a dominant packing material, has impacted our lives since the 1960s with its global consumption reaching over 24 million tons per year. The present common practice of PET waste landfilling has led to serious environmental problems, and chemical recovery faces a huge challenge as a result of the complexity associated with the recycling methods coupled with low efficiency. On one hand, the current low-value market of the downstream products from recycled PET and the low prices of the virgin PET are the two main factors responsible for the low recycling rate of waste PET in South Africa. The PET recycling industry requires new processes to gain more value out of the PET wastes. On the other hand, governmental sectors in different countries have started to set penalties on non-recycled plastics, for instance, France has created a new penalty system where items packaged in non-recycled plastic could cost up to 10% more, and taxes on rubbish buried in landfills will also be increased. In this regard, an attractive and high-value recycling option for depolymerising PET bottles to obtain terephthalic acid (BDC) which is used as a linker for producing high value metal-organic frameworks (MOFs) has been demonstrated (Figure 1) as a promising PET recycling strategy.

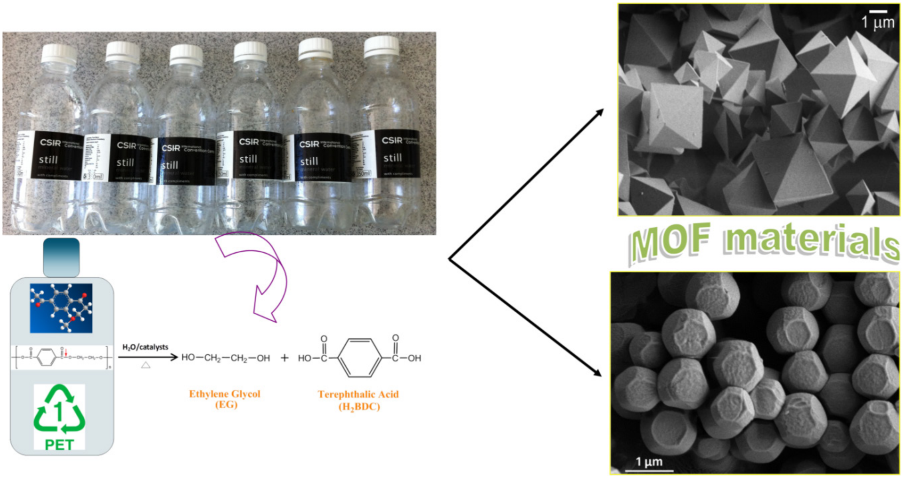


Figure 1: Conversion of waste PET into high value-added MOFs materials

MOFs as a new generation of porous materials are expected to solve real problems and challenges, and offer better performance than conventional materials, such as zeolites and activated carbons. MOFs have been reported to have wide industrial applications, such as gas storage, separation, purification, catalyst, sensor, drug delivery, etc. Although many bench scale experimental work on MOFs synthesis has been conducted, the biggest barrier to their wide-scale commercialisation has been due to the high cost of the constituent chemical feedstocks, of which the organic linkers are the most expensive. Therefore, for MOFs to advance towards large-scale commercial production and applications, there is a need to develop production technologies that will reduce their cost. In this regard, funded by the South African Department of Science and Innovation (DSI) HySA Infrastructure programme, the Council for Scientific and Industrial Research (CSIR) has built up the capabilities to develop the synthesis strategies for different types of MOFs. Of particular interest, our studies have shown that it is possible to produce high quality MOFs, such as those containing Cr, Fe and Zr metal centre. The developed MOFs (UiO-66, MIL-101-(Fe), MIL-101(Cr)) are known for their attractive properties and are applicable in many industrial processes.

The initial focus of our research was on the use of clear PET bottles and work was conducted on a small-batch scale level. Coloured bottles and food PET trays are currently considered as a problematic PET waste stream in South African PET recycling industries. Therefore, our preliminary research experiments proved successful with regards to the depolymerisation process of coloured bottles and food PET trays as well as MOFs synthesis. To complete the evaluations and leverage, the high potential for PET recycling into high-valuable MOF materials, there is a need to conduct further focussed research that integrates all aspects of PET-to-MOFs recycling technology so as to facilitate decision-making for the pre-commercialisation phase. In order to advance the proof of concept and move PET-to-MOF technology towards commercialisation, there is also a need to conduct a techno-economic feasibility study on the viability of converting waste PET to MOFs. In such a manner, the requisite information for making important decisions can be derived in the transition of the research towards the pre-commercialisation phase.

This work aims to review the proposed solution, and determine if the business idea of PET-to-MOFs has a potential of success by taking into account the technical feasibility, economical appraisal, commercial viability, and risk assessment. In the course of the project implementation, a process model was developed to cover the mass balance, which considered material flows, chemical build-up, and energy requirements. The balance was based on a case of 1 kg/batch, and the scalability was proved at a later stage. A financial model was then developed to analyse the economic appraisal and commercial viability.

The result of this study will provide sufficient information and reveal whether this technology is worth further investment. More importantly, the outcomes of this study would provide the government sectors and other stakeholders with sufficient information to serve as a basis for consideration of this business model for increasing the current recycling/reprocessing of waste PET in South Africa.

2. Methodology

2.1. KG-scale depolymerisation of coloured PET bottles and PET food trays

A laboratory-scale crusher (model PC-180) was used to crush the coloured PET bottles and PET food trays (Figure 2a). Then a solvothermal approach was employed to depolymerise the coloured PET bottles and PET food trays in a 5 L high-pressure reactor as shown in Figure 2b. The following is the typical procedure:

1. The coloured PET bottles (green and brown) and PET food trays were collected and cleaned. Bottle caps, rings, and labels were removed accordingly.
2. The cleaned coloured PET bottles and PET food trays were crushed using the above-mentioned crusher.
3. The crushed waste PET (coloured PET bottles and PET food trays) and the calculated amount of water were put into the reactor.
4. The reactor was heated up to a temperature of 200 °C and maintained for 8 to 20 h at an autogenous pressure.
5. The solid product was separated from the mother liquid by centrifugation and dried after being washed twice in N,N-dimethylformamide (DMF).

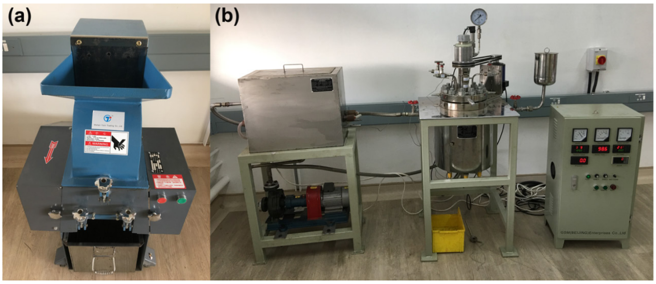
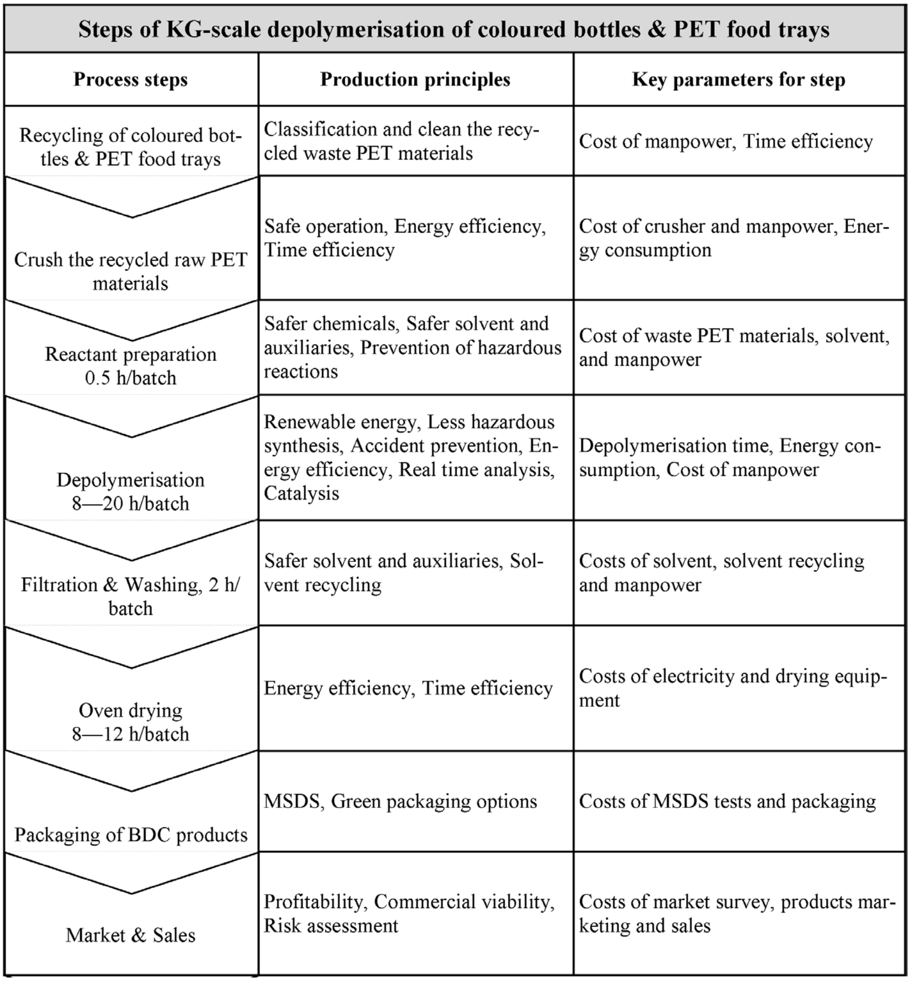


Figure 2: Digital pictures of: (a) Crusher for PET bottles, and (b) the 5 L reactor used in this project

The deploymerisation process for the baseline cost assessment is defined in Figure 3.



Steps of KG-scale depolymerisation of coloured bottles & PET food trays		
Process steps	**Production principles**	**Key parameters for step**
Recycling of coloured bottles & PET food trays	Classification and clean the recycled waste PET materials	Cost of manpower, Time efficiency
Crush the recycled raw PET materials	Safe operation, Energy efficiency, Time efficiency	Cost of crusher and manpower, Energy consumption
Reactant preparation 0.5 h/batch	Safer chemicals, Safer solvent and auxiliaries, Prevention of hazardous reactions	Cost of waste PET materials, solvent, and manpower
Depolymerisation 8—20 h/batch	Renewable energy, Less hazardous synthesis, Accident prevention, Energy efficiency, Real time analysis, Catalysis	Depolymerisation time, Energy consumption, Cost of manpower
Filtration & Washing, 2 h/batch	Safer solvent and auxiliaries, Solvent recycling	Costs of solvent, solvent recycling and manpower
Oven drying 8—12 h/batch	Energy efficiency, Time efficiency	Costs of electricity and drying equipment
Packaging of BDC products	MSDS, Green packaging options	Costs of MSDS tests and packaging
Market & Sales	Profitability, Commercial viability, Risk assessment	Costs of market survey, products marketing and sales

Figure 3: Process steps, production principles and key parameters of KG-scale deploymerisation of the coloured PET bottles and PET food trays (MSDS - Material Safety Data Sheets)

2.2. Deduced industrial-scale depolymerisation of coloured PET bottles and PET food trays

With the know-how of the laboratory-scale depolymerisation of coloured PET bottles and PET food trays, the industrial-scale depolymerisation can be deduced based on the assumptions below: firstly, the de-labelling, cleaning, and crushing processes of the recycled PET raw materials can be combined with higher energy efficiency, time efficiency, and higher automation. The reactor used to depolymerise the recycled PET materials will have big capacity with higher volume availability, energy efficiency as well as time efficiency. At the industrial-scale process, the depolymerisation process can be standardised to take 8 h. The filtration, solvent recycling and vacuumdrying steps can be combined. This combination has the potential to shorten the total filtration, solvent recycling, washing, and drying time from 16 h to 4 h. A comparison of generalised laboratory-scale deploymerisation conditions and our assumed industrial-scaledeploymerisation conditions is summarised in Table 1.

Table 1: Laboratory-scale vs Industrial-scale deploymerisation conditions

Process steps	**Unit**	**Laboratory values**	**Industrial assumptions**
Deploymerisation rate	%	85	85
Raw material	/	Waste PET	Waste PET
Solvent	/	Water	Water
Reactor autogenous pressure	bar	2	2
Reactor temperature	°C	200	200
Reaction time	h	12	8
Washing times	/	4	4
Wash fluid	/	DMF/methanol	DMF/methanol
Recycling	%	90	90
Drying time	h	12	4
Powder loss during processing	%	5	5

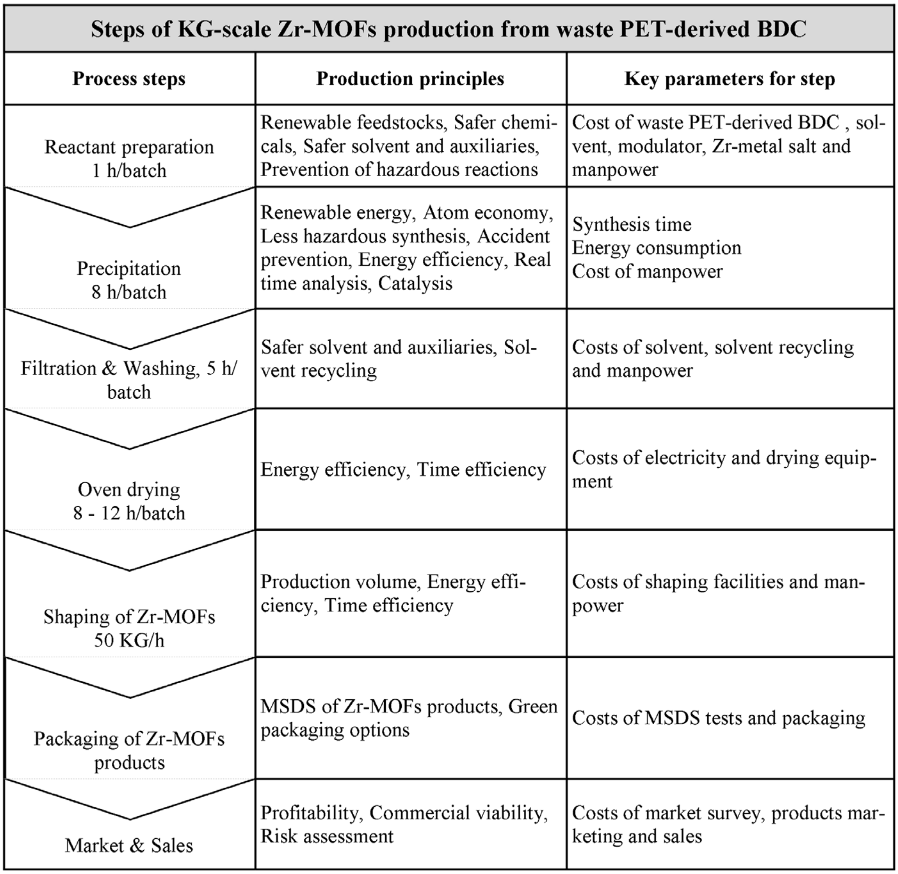
2.3. KG-scale of MOFs synthesis

The same laboratory-scale solvothermal synthesis was used to produce KG-scale MOF UiO-66(Zr) in a 5 L high-pressure reactor. The process steps were as follows:

1. The waste PET (coloured PET bottles and PET food trays)-derived BDC and Zr-metal salt were put into the reactor.

2. The calculated amount of DMF was poured into the reactor as a solvent.
3. The calculated amount of formic acid was poured into the reactor as a modulator.
4. MOF UiO-66(Zr) materials were obtained after 8 h at an elevated temperature of 120 °C and an autogenous pressure.
5. The MOF UiO-66(Zr) products were separated from the mother liquid by centrifugation.
6. Products were washed twice in methanol and dried after being separated from the solvents.

The production process for the baseline cost assessment for the representatitve MOF UiO-66(Zr) is defined in Figure 4.



Steps of KG-scale Zr-MOFs production from waste PET-derived BDC

Process steps	Production principles	Key parameters for step
Reactant preparation 1 h/batch	Renewable feedstocks, Safer chemicals, Safer solvent and auxiliaries, Prevention of hazardous reactions	Cost of waste PET-derived BDC , solvent, modulator, Zr-metal salt and manpower
Precipitation 8 h/batch	Renewable energy, Atom economy, Less hazardous synthesis, Accident prevention, Energy efficiency, Real time analysis, Catalysis	Synthesis time Energy consumption Cost of manpower
Filtration & Washing, 5 h/batch	Safer solvent and auxiliaries, Solvent recycling	Costs of solvent, solvent recycling and manpower
Oven drying 8 - 12 h/batch	Energy efficiency, Time efficiency	Costs of electricity and drying equipment
Shaping of Zr-MOFs 50 KG/h	Production volume, Energy efficiency, Time efficiency	Costs of shaping facilities and manpower
Packaging of Zr-MOFs products	MSDS of Zr-MOFs products, Green packaging options	Costs of MSDS tests and packaging
Market & Sales	Profitability, Commercial viability, Risk assessment	Costs of market survey, products marketing and sales

Figure 4: Process steps, production principles and key parameters of KG-scale MOF UiO-66(Zr) production from waste PET-derived BDC.

2.4. Deduced industrial-scale MOFs production

An industrial-scale MOFs production from the waste PET was deduced based on the reaction conditions and process steps demonstrated at a laboratory scale as described above. However, based on engineering judgement, the laboratory procedures are not suitable for high production rates, so some variations on the laboratory procedures need to be examined as the Industrial Baseline Process. The process' steps, production principles, and key parameters are listed accordingly. This process is based on laboratory-scale synthesis but has been modified to translate the steps to standard operations conducted in large production facilities. Thus, the Industrial Baseline Process is intended to represent the cost if the proven laboratory-scale synthesis were transferred directly to scale-appropriate unit operations. This section will describe the assumptions that were made to scale up laboratory-demonstrated synthesis.

At the industrial-scale production, it is assumed that the reaction temperature can be raised to 160 °C to shorten the reaction time from 8 h to 6 h and improve the yield of the MOF UiO-66(Zr) products. The filtration, drying and vacuum activation steps can be combined using a rotary dryer, which has the potential to shorten the total washing and driving time from 16 h to 6 h, and meanwhile remove the excess organic ligands that might remain in the framework pores after the filtration/wash step. This contaminant cleaning effect is expected to be more effective than that achievable in a spray dryer or belt dryer due to the much longer residence time at temperature. A comparison of generalised laboratory-scale solvothermal reaction conditions and our assumed industrial-scale solvothermal reaction conditions are summarised in Table 2. Zr-metal precursors and reaction modulators were generally selected for scale-up from demonstrated laboratory-scale solvothermal synthesis.

Table 2: Laboratory-scale vs Industrial-scale Process Conditions

Process steps	**Unit**	**Laboratory values**	**Industrial assumptions**
Molar yield	%	85	85
Metal salt	/	$ZrCl_4$	$ZrCl_4$
Organic linker	/	Waste PET-derived BDC	Waste PET-derived BDC
Waste PET-derived BDC: metal salt molar ratio	/	0.5:1	1:1
Solvent	/	DMF	DMF

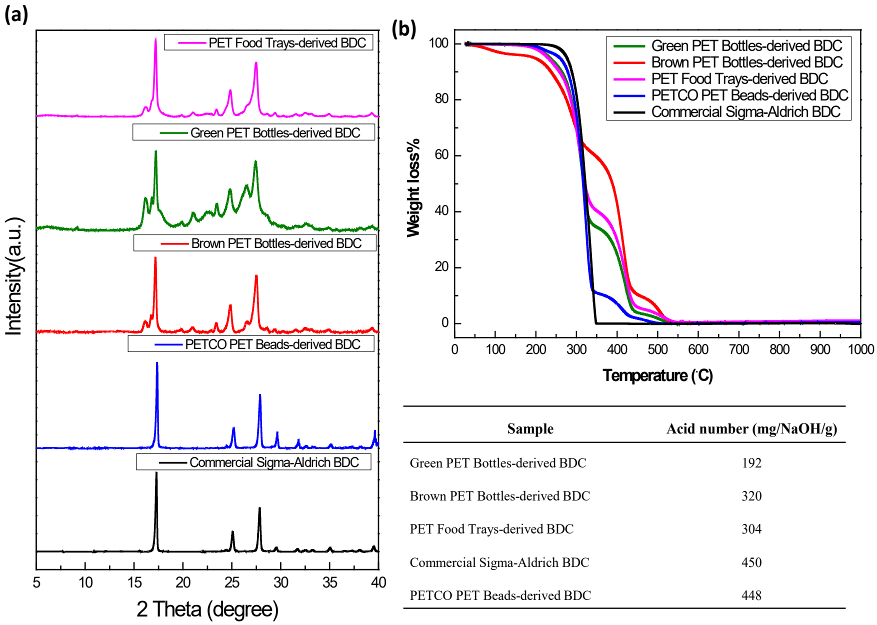
Process steps	**Unit**	**Laboratory values**	**Industrial assumptions**
Modulator	/	Formic acid	Formic acid
Reactor autogenous pressure	bar	1	1
Reactor temperature	°C	120	160
Reaction time	h	8	6
Washing times	/	4	2
Wash fluid	/	methanol	methanol
Recycling	%	90	90
Drying time	h	12	4
Powder loss during processing	%	5	5

The above are expected to be valid assumptions because of the similarities between the laboratory-scale and industrial-scale process conditions of producing MOF UiO-66(Zr) products.

2.5. Technical feasibility of converting coloured waste PET and food trays to BDC

In the experimental trials, different PET sources including green PET bottles, brown PET bottles, PET food trays, and PETCO PET beads were converted to BDC products. Meanwhile, the characterisation results of the derived-BDC samples were compared with those of the commercial BDC purchased from Sigma-Aldrich, as illustrated in Figure 5.

Figure 5a shows the X-ray diffraction (XRD) patterns of the BDC products from different PET sources. Compared to the commercial Sigma-Aldrich BDC sample with a purity of 98%, the crystallinity of PETCO PET Beads-derived BDC is very close to that of the commercial BDC, as evidenced by the similar acid number of 448 mg NaOH/g against 450 mg NaOH/g. As indicated by the XRD patterns, the crystallinity of the Brown PET Bottles derived-BDC sample is similar to that of the PET Food Trays-derived BDC sample, and the containing acid numbers are also nearly the same. In contrast, the crystallinity of the Green PET Bottles-derived BDC is the lowest, with an acid number of only 192 mg NaOH/g. It can be seen from Figure 5b that the purities of the different BDC samples are slightly different.



Sample	Acid number (mg/NaOH/g)
Green PET Bottles-derived BDC	192
Brown PET Bottles-derived BDC	320
PET Food Trays-derived BDC	304
Commercial Sigma-Aldrich BDC	450
PETCO PET Beads-derived BDC	448

Figure 5: (a) PXRD patterns, and (b) TGA curves of the BDC samples derived from different PET sources. Right bottom Table: the titration results of the acid numbers from different BDC samples

2.6. Technical feasibility of converting coloured waste PET and food trays-derived BDC to MOF UiO-66(Zr)

Several characteristic reflection signals in Figure 6a confirmed the successful synthesis of MOF UiO-66(Zr) from different PET-derived BDC when compared to the simulated XRD pattern. The relative crystallinities of the obtained MOF UiO-66(Zr) samples are comparable to that from commercial BDC feedstock from Sigma-Aldrich. However, the Zr-MOF sample synthesised from Green PET Bottles-derived BDC shows the lowest relative crystallinity. The scanning electron microscope (SEM) images in Figure 6b-f show the quite different morphologies of the obtained MOF UiO-66(Zr) samples.

Figure 7a shows the thermogravimetric analysis (TGA) properties of the obtained MOF UiO-66(Zr) prepared from different BDC sources. The N_2 and H_2 sorption isotherms presented in Figure 7b, respectively, indicate that all the PET-derived MOF UiO-66(Zr) materials have relatively lower N_2 and H_2 adsorption levels, but the obtained values (as listed at the bottom of Figure 7b) are comparable to that from the commercial feedstock as well as other previously developed MOF UiO-66(Zr) materials. As MOF

UiO-66(Zr) samples were also synthesised from the coloured PET bottles-derived BDC, where the effects of additives and colourants should be taken into account on the textural properties of the prepared MOF UiO-66(Zr). The experimental results suggested that the MOF UiO-66(Zr) samples from the clear PET food trays-derived BDC have lower textural properties than those from a clear PET beads-derived BDC. The reason could be the effects of additives and colourants from the green and brown coloured bottles.

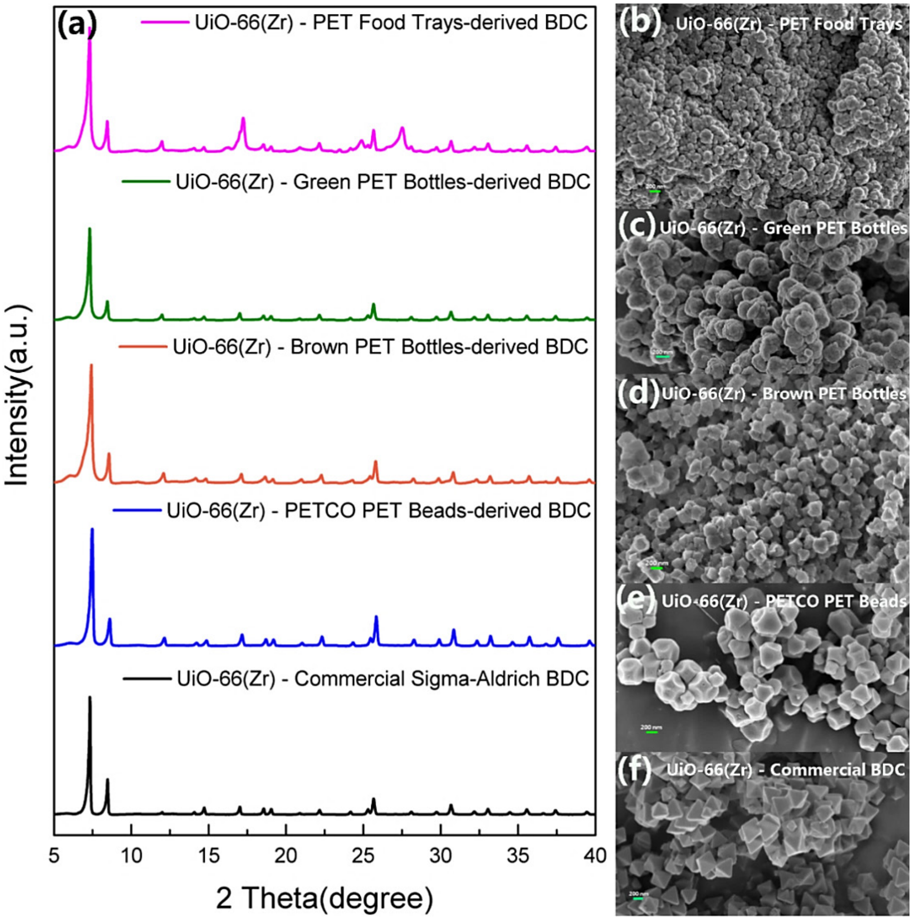


Figure 6: (a) XRD patterns and (b-f) SEM images of the Zr-MOF samples prepared from different BDC sources

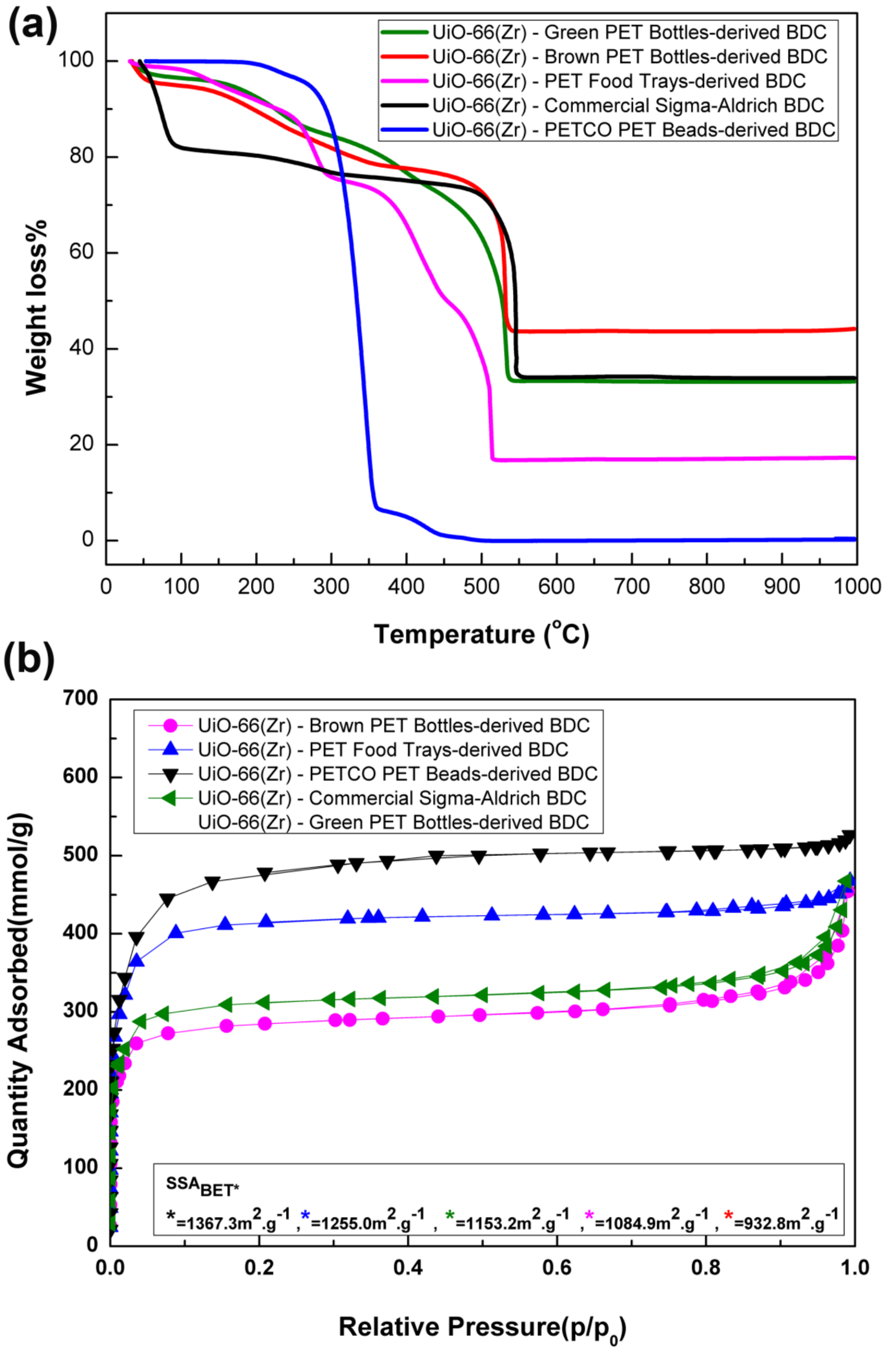


Figure 7: (a) TGA curves and (b) N_2 sorption of the MOF UiO-66(Zr) samples prepared from different BDC sources. Bottom: BET and H_2uptake results of the prepared MOF UiO-66(Zr) samples

2.7. Economic appraisal and commercial viability on the business model: converting coloured waste PET and food trays to MOFs

2.7.1 Costing factors and assumptions in KG-scale

The cost results of KG-scale depolymerisation of coloured bottles and PET food trays are presented in Table 3.

The cost was calculated based on the respective materials, process conditions, and times presented in Figure 4. For the KG-scale experiments on depolymerisation of the waste-coloured bottles and food trays, the samples were 'home collected' by the researchers. The costs of chemicals were calculated based on the usage and prices available on the Sigma-Aldrich website. The cost of electricity was calculated based on the Eskom charges of R1.94/kWh. The cost of labour was calculated based on the rate of a PhD candidate working at the CSIR. The market price for waste PET-derived BDC was referred to as the commercial BDC price. In Table 3, material costs reflect the costs of raw materials (recycled PET, solvents and additives), while manufacturing costs reflect the cost of machinery amortised over equipment lifetime as well as process energy, utilities, labour, and facility costs. As seen, the machinery costs dominate the total costs for the KG-scale depolymerisation of coloured bottles and PET food trays to produce BDC. Apparently, the profitability of this case is very low, and there is potential to lower the manufacturing costs by scaling-up the process. The cost results of KG-scale MOF UiO-66(Zr) production from waste PET-derived BDC trays are presented in Table 4**.**

MOF UiO-66(Zr) product serves as a representative MOF to illustrate cost trends. Costs are divided between materials and manufacturing costs and are further segregated by the processing steps shown in Figure 5. The cost was calculated based on the respective materials, process conditions, and times.

For the KG-scale experiments of Zr-MOF production, the BDC acid was derived from the recycled coloured bottles and food trays in the previous step. The costs of chemicals were calculated based on the usage and prices available on the Sigma-Aldrich website (on 25 March 2019). The cost of electricity was calculated based on the Eskom charges of R1.94/kWh. The cost of labour was calculated based on the rate of estimated labour h (based on an hourly rate of a salary of R500k annually) for three technicians requested. A levelised price of ZAR198240/kg was taken by averaging the prices of several available MOFs products in Table 5. However, a late quotation on MOF UiO-66(Zr) was received from Strem Chemicals Inc. at ZAR283, 638/kg, and the formal quotation sheet was attached in Annexures (II). In Table 4, the material costs reflect the costs

Table 3: Cost calculations of KG-scale depolymerisation of coloured bottles and PET food trays

	Facilities		Raw materials		Cost of electricity (ZAR)*	Cost of labour (ZAR)#	Sub-Total (ZAR)
Process steps	**Description**	**Cost (ZAR)**	**Description**	**Cost (ZAR)&**			
Recycling of coloured bottles & PET food trays	-	-	-	-	-	200	**200**
Crush the recycled raw PET materials 0.5 h/batch	Crusher	32,000	-	-	4	65	**32,069**
Reactant preparation 0.5 h/batch	-	-	D.I H_2O	100	-	65	**165**
Depolymerisation 8 - 20 h/batch	5L reactor	200,000	Ethylene glycol	368	14	1,040	**202,665**
			D.I H_2O	100	103	1,040	
Filtration & Washing, 3.5 h/batch	Overhead stirrer	11 264	D.I H_2O	100	0.48	455	**29,219**
	Vacuum pump	14 500	Filter paper	2900	0.40		
Oven drying 8 - 12 h/batch	Oven	15,000	-	-	14	1040	**16,054**
Yield of BDC (kg)							**1**
Market Price (ZAR/kg)							**2,000**
Cost as per Sigma Aldrich website; *Calculations based on Eskom charges = R1.94/kWh; #Calculations based on CSIR's PhD Candidate rates = R130/h							

Table 4: Cost calculations of KG-scale MOF UiO-66(Zr) production from waste PET-derived BDC

Process steps	Facilities		Raw materials		Cost of electricity (ZAR)	Cost of labour (ZAR)	Sub-Total (ZAR)
	Description	**Cost (ZAR)**	**Description**	**Cost (ZAR)**			
Reactant preparation, 1 h/batch	Sonicator bath	9,430	D.I H_2O	100	13	130	**9,673**
Precipitation, 5 h/batch	Hot plate/ Magnetic stirrer	2,000	$ZrCl_4$	536	8	650	**210,474**
			PET-derived BDC	2,000			
	5L reactor	200,000	Formic acid	1,614	64	650	
			DMF	2,960			
Filtration & Washing, 5 h/batch	Centrifuge	68,000	Conical centrifuge tubes	50	1	65	**72,173**
			D.I H_2O	100			
	Hot plate/ Magnetic stirrer	2,000	Paraffin liquid	99	8	650	
			Ethanol	1200			
Oven drying 8-12 h/batch	Oven	15,000	-	-	14	1,040	**16,054**
Yield of Zr-MOF (kg)							**1**
Market Price (ZAR/kg)*							**198,240**

*Average price took from Sigma-Aldrich website on MOFs products.

of raw materials (salts, linkers, and solvents), while manufacturing costs reflect the cost of machinery amortised over equipment lifetime as well as process energy, utilities, labour, and facility costs. Still, the machinery costs dominate the entire manufacturing costs for the solvothermal synthesis of the representative MOF UiO-66(Zr). The profitability for this case still reflects negative, and the potential to make a turnover can be expected from the scale-up of the manufacturing process of the representative MOF UiO-66(Zr). This would offer potential cost reductions through the advantage of economies of scale as well as removing a layer of cost mark-up. Material costs also contribute more to the total production cost than manufacturing costs for all cases.

2.7.2. Costing factors and assumptions in 10KG-scale

Table 6 lists the cost calculations of semi-industrial-scale (10KG/day) depolymerisation of coloured bottles and PET food trays, and the following assumptions have been considered: the recycled PET beads will be purchased directly from the local PET recycling companies such as PETCO at approximately R20/ton. Given a depolymerisation rate of 85% and 5% powder loss during processing, to produce 10KG of BDC, 12.5KG recycled PET will be required. As the recycled PET can be delivered in the bead form, there is no need to crush in the laboratory anymore. The size of the reactor will be scaled-up to 50 L, and the prices of the reactants will be at 50% discount compared to the 1KG-scale experiments. The energy efficiency at 10KG-scale production can be improved by 50% compared to the 1KG-scale. The cost of labour will be paid annually at ZAR600,000 in total. When coming to the semi-industrial-scale operation, three employees will be hired, including one for marketing and Sales, a technician, and an accountant with annual salary packages of R310399, R261641, and R282413, respectively.

Table 7 lists the cost calculations of industrial-scale (10KG/day) MOF UiO-66(Zr) production from waste PET-derived BDC, and the following assumptions have been considered: the BDC acid linker will use the waste PET-derived BDC products. A conversion rate of 85% and 5% powder loss during processing was considered to produce 10KG of MOF UiO-66(Zr). The size of the reactor will be scaled-up to 50 L, and the prices of the reactants will be at 50% discount compared to the 1KG-scale experiments. The energy efficiency at 10KG-scale MOF UiO-66(Zr) production can be improved by 50% compared to the 1KG-scale. Regarding the industrial-scale operation, three employees will be hired, including one for marketing and sales, a technician and an accountant with annual salary packages of R310399, R261641, and R282413, respectively.

Table 5: Prices of the example MOFs products from Sigma-Aldrich.

Supplier	**MOFs**	**Synonym**	**Empirical formula**	**Price (ZAR/KG)**	**Note**
Sigma-Aldrich	Basolite® Z1200	2-Methylimidazole zinc salt, ZIF-8	$C_8H_{10}N_4Zn$	186,000	
Sigma-Aldrich	Basolite® F300	Fe-BTC, Iron 1,3,5-benzenetricarboxylate	$C_9H_3FeO_6$	117,600	
Sigma-Aldrich	Basolite® A100	Aluminum terephthalate, MIL-53(Al)	$C_8H_5AlO_5$	174,000	
Sigma-Aldrich	Basolite® C 300	Copper benzene-1,3,5-tricarboxylate, Cu-BTC MOF, HKUST-1	$C_{18}H_6Cu_3O_{12}$	297,600	
Sigma-Aldrich	Basolite® Z377	MOF 177	$C_{54}H_{30}O_{13}Zn_4$	216,000	
Strem Chemicals	Zr-MOF	UiO-66(Zr)	$Zr_6O_4(OH)_4(BDC)_6$	283,638*	USD20000/KG

*The exchange rate was: 1 USD =ZAR14.1815 on 04/04/2019.

Table 6: Cost calculations of semi industrial-scale (10KG/day) depolymerisation of coloured bottles and PET food trays

	Facilities		Raw materials		Cost of electricity (ZAR)*	Cost of labour (ZAR)#	Sub-Total (ZAR)
Process steps	Description	Cost (ZAR)	Description	Cost (ZAR)&			
Recycling of coloured bottles & PET food trays	-	-	-	-	-	200	**200**
Crush the recycled raw PET materials 0.5 h/batch	Crusher	0	-	-	0	0	**0**
Reactant preparation 0.5 h/batch	-	-	D.I H2O	100	-	82	**182**
Depolymerisation 8 h/batch	50L reactor	500,000	E.G.	368	14	1308	**501893**
			D.I H2O	100	103		
Filtration & Washing, 3.5 h/batch	Presser	68,000	Filtration	50	1	573	**68724**
			D.I H2O	100			
	Stirrer/ Heating block	2,000	Paraffin liquid	99	5		
Oven drying 8 - 12 h/batch	Oven	15,000	-	-	14	0	**15014**
Packaging of BDC products	-	-	Plastic bags	20	-	130	**150**
Yield of BDC (KG)							**10**
Market Price (ZAR/KG)							**2,000**
&Cost as per Sigma Aldrich website; *Calculations based on Eskom charges = R1.94/kWh; #Calculations based on CSIR's PhD Candidate rates = R130/h							

Table 7: Cost calculations of semi- industrial-scale (10KG/day) MOF UiO-66(Zr) production from waste PET-derived BDC

Process steps	Facilities		Raw materials		Cost of electricity (ZAR)	Cost of labour (ZAR)	Sub-Total (ZAR)
	Description	Cost (ZAR)	Description	Cost (ZAR)			
Reactant preparation, 1 h/batch	Sonicator bath	9,430	D.I H_2O	100	13	163.5	**9,673**
Precipitation, 8 h/batch	Stirrer/heating block	2,000	$ZrCl_4$	536	8	1308	**510,474**
			PET-derived BDC	2,000			
	50L reactor	500,000	Formic acid	1,614	64		
			DMF	2,960			
Filtration & Washing, 5 h/batch	Vacuum filtration system	68,000	Conical centrifuge tubes	50	1	817.5	**70,973**
			D.I H_2O	100			
	Stirrer	2,000	Paraffin liquid	99	8		
Oven drying 8-12 h/batch	Oven	15,000	-	-	14	0	**16,054**
Yield of Zr-MOF (KG)							**10**
Market Price (ZAR/KG)*							**198,240**

2.7.3. Financial Viability

The theory of financial viability measures two outputs, namely;

- Financial profitability and solvency of the planned investments
- The viability of a new project or enterprise.

A sound investment is one that generates enough revenue to meet all financial obligations on a timely basis and command an adequate level of working capital for continued operations. Usually, it implies the ability to earn a reasonable rate of return on capital employed. The extent of the success of a project is determined by a review of its financial structure, liquidity trends, and profitability over time. For a new project, the main objective of the analysis is to demonstrate that the financial cash flows expected to be generated are attractive to prospective investors, encouraging them to contribute equity funds to the particular project rather than to employ them elsewhere. Contributing equity investments to a project lessens the burden of raining project finance. Development financial institutions generally fund projects that are co-financed through an equity investment. The analyses on which investment decisions are based are driven by the net present value (NPV) and the internal rate of return (IRR).

$$NPV = \sum_{t=0}^{n} \frac{Rt}{(1+i)^t}$$

The NPV method consists of discounting all future cash flows to the present value by means of some appropriate rate of interest. The rate of interest to be used should reflect the minimum rate of return which is acceptable to the firm for a given investment. It works on the simple but fundamental principle that an investment is worth undertaking only if the present value of the cash inflows is at least equal to, if not greater than the present value of the cash outflows arising from an investment. To put it another way, companies should make investments in projects with a zero or positive net present value. The calculated NPV for this study is shown in Table 8.

Table 8: Net Present Value for the MOFs project

Year	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029
Index	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Subsidies	0										
Equity	130439										
Private Withdrawal											
Loan	521755										
Total Investment Payout	652194										
CASH POSITION	236400	1286315	998916	1051663	1106213	1166277	1229912	1303203	1391078	1505309	1670124
Cash position cumulated; negative values compensated by current account	236400	1049915	2048831	3099895	4206108	5371385	6601297	7904500	9295578	10800887	12471012
Cash Flow after Dept Service, after tax	236400	1266315	998916	1051063	1106213	1165277	1229912	1303203	1391078	1505309	1670124
Cash Flow after Dept, before tax	236400	1641502	1373085	1445148	1521316	1602803	1691814	1792452	1912590	2067839	2308548
Equity	130439										
Free Cash-Flow (before tax) to Equity	366839	1641502	1373085	1445148	1521316	1602803	1691814	1792452	1912590	2067839	2308548

Table 9: IRR and NPV to equity

Year		**2019**	**2020**	**2021**	**2022**	**2023**	**2024**	**2025**	**2026**	**2027**	**2028**	**2029**
Index		**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
IRR to EQUITY	4.35%											
Free Cash-Flow to Equity		366839	1641502	1373085	1445148	1521316	1602803	1691814	1792452	1912590	2067839	2308548
Benchmark Discounting after 2019		1	0.91	0.83	0.75	0.68	0.62	0.56	0.51	0.47	0.42	0.39
Free Cash-Flow to Equity, discounted to 2019		366839	1492275	1134781	1085761	1039079	996215	954985	919811	892237	876966	890045
NPV to EQUITY	(R20082.31)											
Auxilliary Calculation/Loan	Debt as at 01.01.	521755	474323	426891	379458	332026	284594	237161	189729	142297	94865	47432
	Debt as at 31.12.	474323	426891	379458	332026	284594	237161	189729	142297	94865	47432	0
	Interests as at 31.12.	52176	47432	42689	37946	33203	28459	23716	18973	14230	9486	4743
	Repayment as at 31.12.	47432	47432	47432	47432	47432	47432	47432	47432	47432	47432	47432
Auxilliary Calculation/ Depreciation	Investment/ years	0	0	0	0	0	0	0	0	0	0	0
	Investment/ 10 years	65219	65219	65219	65219	65219	65219	65219	65219	65219	65219	0
	Repayment Investment/ 5 years	0	0	0	0	0	0	0	0	0	0	0
	Total	65219	65219	65219	65219	65219	65219	65219	65219	65219	65219	0

$$IRR = NPV = \sum_{t=1}^{T} \frac{C_t}{(1+r)^t} - C_0 = 0$$

An investor would be interested in the IRR after tax which he would compare with returns from alternative investment opportunities at similar risk levels before committing funds to a particular project. If the IRR after the tax of a project is greater than the cost of capital, it can be concluded that the project is financially viable. Besides, the production machinery is to recover funds and the terms of repayment loans have to be adjusted to take any cash flow requirements. IRR does not provide any information on the requirements for phasing short-term bridging finance or grace periods on the loan required to accommodate delayed benefits. As shown in Table 9, the calculated IRR for producing MOFs in this study is estimated at 4.35% with the assumption of 5.5 annual increases. An annual increase cost of 7.5% on the products offer an IRR of 4.49%.

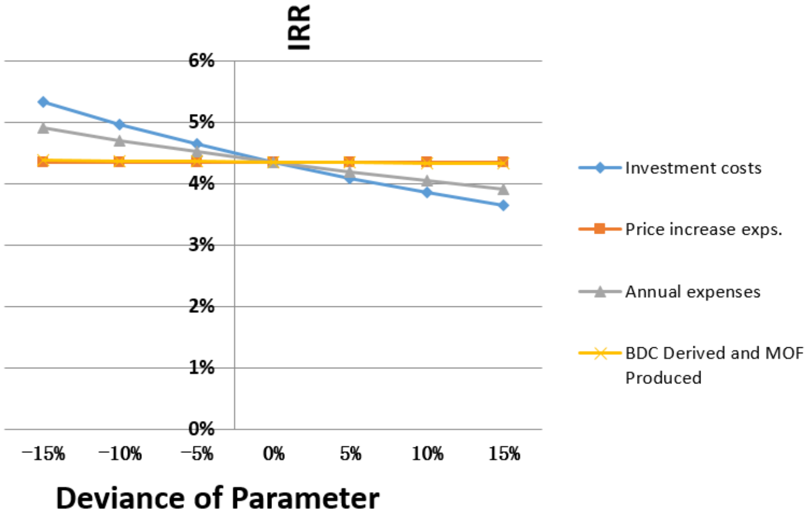


Figure 8: Estimated internal rate of return

Figure 8 shows the estimated internal rate of return. The investment expenditures, including the incremental working capital needs of a project/enterprise need to be met on a well-timed basis with a minimum cost. In setting up the financing plan, consideration for the most effective capital cost requirement is decided in order to satisfy the financial requirements of the business. These requirements are carefully determined by budgeting forecasts as a mechanism to avoid extreme expenditure and over- or under-capitalisation. In a continuing business where a budgetary control system is in operation, the forecasting of requirements presents no difficulty. For new projects, more has to be left to estimates. While costs can be estimated, the generated revenue is solely dependent on demand, which, in turn, is influenced by a number of economic indicators, such as the domestic economic performance that is independent of any business operations. In both new and existing businesses, funds may be raised from external sources but in a continuing business, internal resources can be mobilised by reinvesting profits.

Certain factors need to be taken into account when external financing is considered. These include, a Memorandum of Agreement (MoA) that might be in place before a project funding is concluded, the projected financial condition and performance of the investment, and the inherent risk of business operations. The nature of the need for funds influences the type of financing that should be used. If there is a seasonal component to the business, it offers itself to short-term financing and bank loans in particular. The financial condition and performance of the plant will influence the type of financing that should be utilised. The larger the liquidity position of a plant, the stronger the overall financial condition and the greater the profitability of the firm. On the contrary, the basic business risk faced by any plant has an important bearing on the type of financing that should be used. The desirable debt financing usually becomes less relative to equity financing when the business risk is greater. Equity financing is safer in that there is no contractual obligation to pay interest and repay the principal as there is with a loan.

2.7.4. The financial and economic analysis

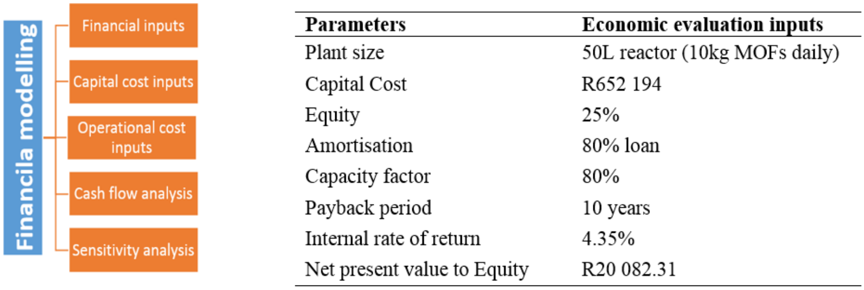
Two ways are used to assess the desirability of undertaking a project: financial and economic analysis. These primary tools are used for carrying out financial and economic analyses, and both types of analyses are required for project screening and selection. However, there is a difference in application since financial analysis deals with the cost and benefit flows from the point of view of a plant's financial viability while economic analysis deals with the costs and benefits to society. In this instance, PET waste would have other climate and social negative impacts. Economic analysis, in this regard, takes a broader view of costs and benefits as well as financial analysis. The methods, nonetheless, differ in several important ways. An enterprise is interested in financial profit and the stability of that profit, while society or government is concerned with much wider objectives such as waste management new economic opportunities, poverty alleviation, and resulting net benefits to society as a whole. Therefore, the objectives of the two types of analysis are different. The cost-benefit analysis for the purposes of this study has not been quantified. Only a financial analysis for a project plant that would produce MOFs has been considered. This means that the cost of landfilling PET waste has not been measured and the potential incomes stream for climate change mitigation have not been calculated.

2.7.5. MOFs financial modelling results

Production costs have been evaluated by adding up fixed costs (depreciation rates), operating and maintenance (O&M), and variable operating and maintenance (VOMs). Data utilised have been collected from literature sources and calculations for the infrastructure energy and water usage have been estimates using utility tariffs, respectively. The estimation of capital investment cost comprised seven parameters that represent the total cost of the infrastructure. The combined parameters for the balance sheet are as follows:

- Crusher
- Overhead stirrer
- Vacuum Pump
- Oven
- Sonicator bath
- Hot plate/Magnetic stirrer
- Centrifuge

These assets have a total capital cost of **R652 194**. The estimated revenue from a 10kg MOF production is **R1 585 920** with additional revenue from PET-derived BDC that is approximately **R2000** per kg. The operations and maintenance costs have been considered as a percentage of capital cost that is shown in Figure 9. The variable fixed operations and maintenance have been represented by 2.5% of the capital cost.



Parameters	Economic evaluation inputs
Plant size	50L reactor (10kg MOFs daily)
Capital Cost	R652 194
Equity	25%
Amortisation	80% loan
Capacity factor	80%
Payback period	10 years
Internal rate of return	4.35%
Net present value to Equity	R20 082.31

Figure 9: Modelling input and results

The calculated financial results from the data shown in Figure 10 are based on a yearly production of MOFs and the derived BDC that generates a total revenue of **R1 601 920**. The cost of the depreciation rate has an impact of **R65 2193** per annum for MOFs produced. Figure 11 shows the different parameters utilised into the overall MOFs production costs. Under the above assumption, the production cost is estimated to be **R270 286** for 10kg of MOFs produced.

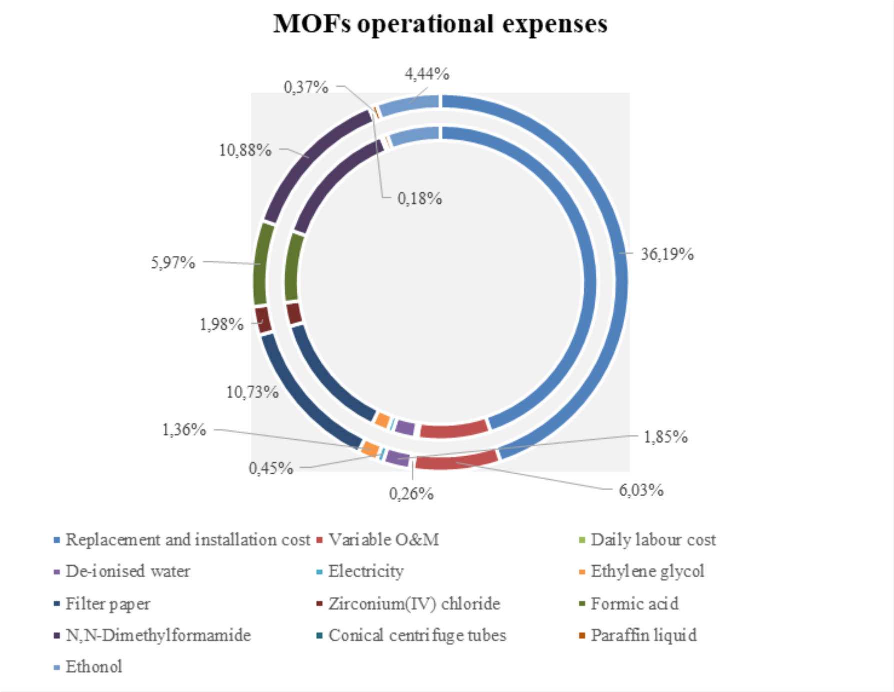


Figure 10: MOFs operational expenses

The depreciation of this evaluation was evaluated over ten years for this plant, while the amortisation estimates have been calculated over a duration of 11 years with a 10% interest rate. This is equivalent to the South African lending rate. The operational expenses show that about 36% of the OPEX cost is used for replacement parts and this is followed by electricity and N,N-Dimethylformamide costs that are about 11% of the operational costs.

Table 10: Revenue generated

Revenue Parameters	
MOFs UiO-66(Zr)	R1 585 920
PET-derived BDC	R16 000

The revenue generated per annum is shown in Table 10 while escalation rates are shown in Figure 11**.** The revenues from produced MOFs show an overall escalation rate of approximately 18% over the lifespan of the projects. The investment cost slope is normal and corresponds with initial investment costs. The operational costs increase with an estimate of 10% over the project life cycle. This is confirmed on the annual expenses slope shown in Figure 11.

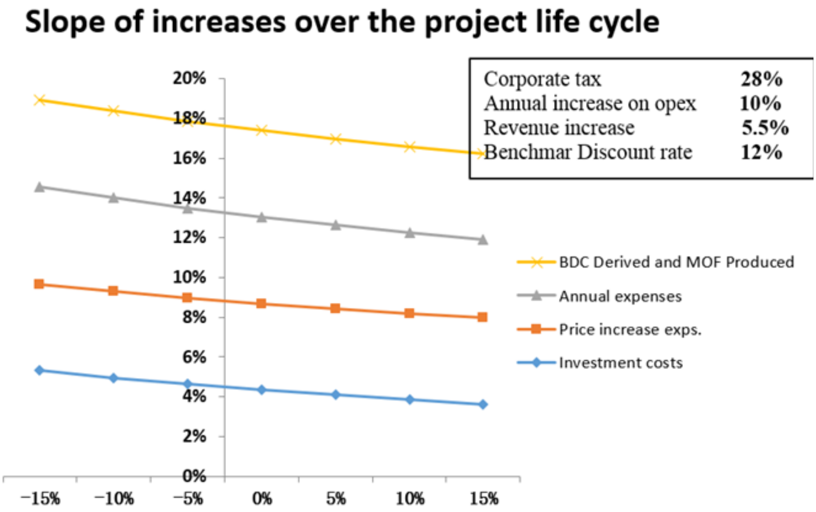


Figure 11: Project costs escalation rate slopes

2.7.6. *Commercial viability*

Investing in MOFs will generate roughly a 5% IRR on a production capacity of 10kg daily. Given the fact that these results are positive at a small-scale, it is therefore recommended that this investment should proceed. The environmental and opportunity cost that is avoided has not been considered in the financial analysis. This can further strengthen the revenue side of this production. While a return of 5% is not the most attractive, the PET waste that would be redirected to this production contributes to the South African waste management strategy and climate change objectives. In addition, the South African government bond of 10 years yields a return of 8.52% return and this initiative is competitiveness with a 5% IRR.

2.8. Risk assessment of converting of coloured waste PET and food trays to MOFs

Table 11. Risks and risk mitigation

Risk	Risk mitigation
Barriers to entry, that is, highly technical expertise on MOFs materials	Employ technical expertise
High set-up costs for a MOF producing facility	Partner with other industries
Engineering knowledge towards the scaling-up of MOFs production	Involve quality chemical engineers
Usage of organic solvents, that is, DMF	Recycle and reuse the organic solvents
Handling and disposal of the hazardous substances	Follow the standard handling and disposal arrangements

As listed in Table 11, the overall assessment of risks and strategies to minimise those risks are provided. The safety, health, and environmental aspects with regards to the handling and disposal of the hazardous substances can be arranged in compliance with national/international standards. There are no other clearances and objection certificates required.

3. Conclusions

This study focused on the coloured bottles and food PET trays as they have been identified as the problematic stream from the current waste PET recycling industries in South Africa.

Firstly, the results of this study revealed the technical feasibilities of lab-scale and KG-scale depolymerisation of coloured bottles and PET food trays to BDC were quite high. The lab-scale and KG-scale production from coloured bottles and PET food trays-derived BDC have also proved technically feasible. The production costs can be significantly reduced at an industrially relevant scale. Given the different BDC-based MOFs, the selection of a manufacturing method will be determined by the suitability of a method for a particular MOF, and it is recognised that a fully continuous synthesis operation has an opportunity to further bring down the production costs. For direct comparison and extension from laboratory-scale, the scope of this analysis was based on a KG-scale batch synthesis with certain steps that could be implemented with a pseudo-continuous operation such as drying and shaping. A future study should be conducted to evaluate each process step to determine the most suitable approach between continuous and batch processing since certain batch process operations may still be optimal. As solvent cost is a significant cost contributor, high solvent recycle rates (≥90%) are crucial to achieving moderate to high-cost projections made within the analysis for solvothermal syntheses. This will be particularly important for MOFs that may not be amenable to aqueous or mechanochemical syntheses. Studies to minimise solvent usage are also recommended. Similarly, a reduction of material costs and sizes of reactors could also contribute in the reduction of MOF manufacturing costs.

Secondly, through the analysis of the built-up financial model, the results of economic appraisal and commercial viability showed that investing in MOFs will generate roughly a 5% IRR on a production capacity of 10kg daily. Given the fact that these results are positive at a small-scale, it is therefore recommended that this investment should proceed. The environmental and opportunity cost that is avoided has not been considered in the financial analysis. This can further strengthen the revenue side of this production. While a return of 5% is not the most attractive, the PET waste that would be redirected to this production contributes to the South African waste management strategy and climate change objectives. In addition, the South African government bond of 10 years yields a return of 8.52% return and this initiative is competitiveness with a 5% IRR.

Finally, the results of this analysis are expected to be generally valid for other BDC-based MOFs from other waste PET materials.

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