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

Technical report: Case Studies

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Waste Research Development and Innovation Roadmap Research Report

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

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EXECUTIVE SUMMARY

In the period of May 2018 – March 2019, the metal-organic Framework (MOFs) Research Group at the CSIR conducted the techno-economic feasibility assessment on the viability of using waste polyethylene terephthalate (PET) (trays and coloured bottles) to produce MOFs. Funding for this project was provided through the Waste RDI Roadmap Grant by the Department of Science and Technology (DST), South Africa. PETCO- the South African PET Recycling Company also provided partial funding support towards the market research part. This is the final report for this project.

MOFs as a new generation of porous materials have been demonstrated into many industrial applications and their performance are much better than those incorporated with conventional materials such as zeolites and activated carbons. However, the high production cost and the availability of the large-scale production approach pose as the two major barriers to prevent MOFs from transitioning laboratory tests to the envisioned applications.

PET as dominant packing materials 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. Particularly, 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 industries require new processes to gain more value out of the PET wastes. In this regard, an attractive and high-value recycling option for depolymerising PET bottles to obtain terephthalic acid (H2BDC) which is used as a linker for producing high value MOFs has been considered as a promising PET recycling strategy. It should be mentioned that this project will focus on the coloured bottles and food PET trays, because they have been identified as the problematic stream from the current waste PET recycling industries in South Africa. The preliminary research experiments had proved success with regards to the depolymerization process of coloured bottles and food PET trays as well as MOFs synthesis. To complete the evaluations and leverage the high potential for the PET recycling into the high-valuable MOF materials, there is a need to conduct further focussed research that integrates all aspect of PET-to-MOFs recycling technology so as to facilitate decision-making for the pre-commercialization phase. The outcomes of this study would provide DST, PETCO 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.

This project reviewed the business model of 'waste PET-to-MOFs' from technical feasibility, economic appraisal, commercial viability, and risk assessment. The following research objectives served as a guide for the research activities:

- Assisted by PETCO/Extrupet, the costs in the process of collection, cleaning as well as the risk of contaminants associated with the dirty nature of the PET reducing the performance and quality of the obtained MOFs were taken into account.
- To scale up the PET-to-MOFs process (1 kg) either in a batch or continuous production process.
- To conduct a techno-economic feasibility study on the viability of converting colored PET bottles and PET food trays to MOFs.
- To highlight several niche and high volume applications of the PET-derived MOF materials.

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 the later stage. The process would produce saleable MOFs products for the South African market.

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% 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, since the South African government bond of 10 years yields a return of 8.52% return, this initiative is competitiveness with a 5% IRR.

TABLE OF CONTENTS

List of Figures

List of Tables

List of Abbreviations

DST: Department of Science and Technology

DOE: Department of Energy (DOE)

CSIR: Council for Scientific and Industrial Research

ECSA: Engineering Council of South Africa

SACNSP: South African Council for Natural Scientific Professions

TUT: Tshwane University of Technology

UiO: University of Oslo

MIL: Materials of the Institut Lavoisier

PETCO/Extrupet: two of the South African PET Recycling Companies

ISE: International Society of Electrochemistry

RSC: Royal Society of Chemistry

R&D: Research and Development

MOFs: Metal-organic Frameworks

PET: Polyethylene terephthalate

BDC: Terephthalic acid

EG: Ethylene glycol

DMT: Dimethyl terephthalate

DMF: N,N-dimethylformamide

MSDS: Material Safety Data Sheets

WP: Breakdown work packages

KC: Key considerations

Kg: Kilogram

XRD: X-ray diffraction

SEM: Scanning Electron Microscope

TGA: Thermogravimetric Analysis

NPV: Net present value

IRR: Internal rate of return

MoA: Memorandum of Agreement

O&M: Operations and maintenance

VOM: Variable operating and maintenance

1. Introduction

1.1 Background

Polyethylene terephthalate (PET), as dominant packing materials, 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 started to set penalties on the 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.

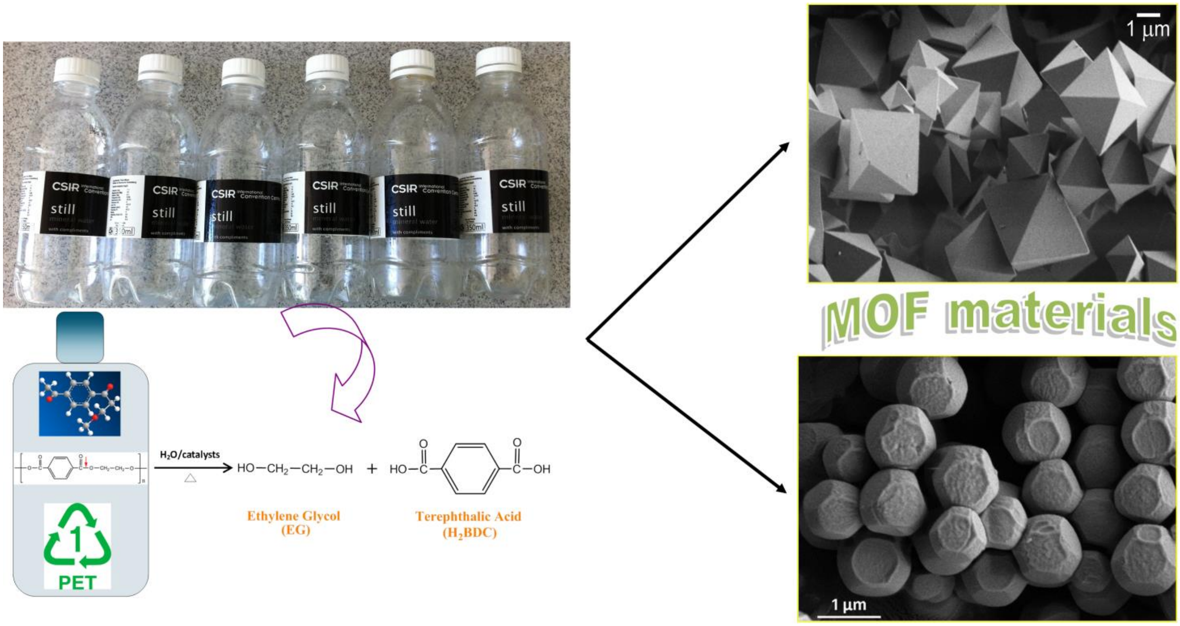


Figure 1: *Convert waste PET into high value-added MOFs materials*

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. MOFs as a new generation of porous materials are expected to solve real problems and challenges with much better performance than conventional materials such as zeolites and activated carbons. The initial focus of our research concentrated on the use of clear PET bottles and the work was conducted on a small-batch scale level. As the coloured bottles and food PET trays are currently considered as the problematic PET waste stream in South African PET recycling industries. In this project, the techno-economic feasibility assessment on the viability of coloured bottles and food PET trays to produce MOFs will be conducted in 2018/19 financial year, and the results will be reported back to DST, PETCO and other stakeholders to facilitate decision-making for the high potential for the PET recycling into the high-valuable MOF materials in South Africa.

1.2 Objectives

This project is to review the proposed solution and determine if the business idea of PET-to-MOFs has a good chance of success by taking into account the technical feasibility, economical appraisal, commercial viability and risk assessment. The result of this study will provide sufficient information and tell whether this technology is worth further investment.

1.3 Research Activities

Under the financial supports, the production process of KG-scale MOFs from waste colored PET bottles and food PET trays will be optimized. The scope and activities of the proposed research are highlighted below.

- Assisted by PETCO/Extrupet, the costs in the process of collection, cleaning as well as the risk of contaminants associated with the dirty nature of the PET reducing the performance and quality of the obtained MOFs will be taken into account.
- To scale up the PET-to-MOFs process (~1 kg) either in a batch or continuous production process.
- To conduct a techno-economic feasibility study on the viability of converting coloured PET bottles and PET food trays to MOFs.
- To highlight several niche and high volume applications of the PET-based MOF materials as shown in the *Figure 2* below.

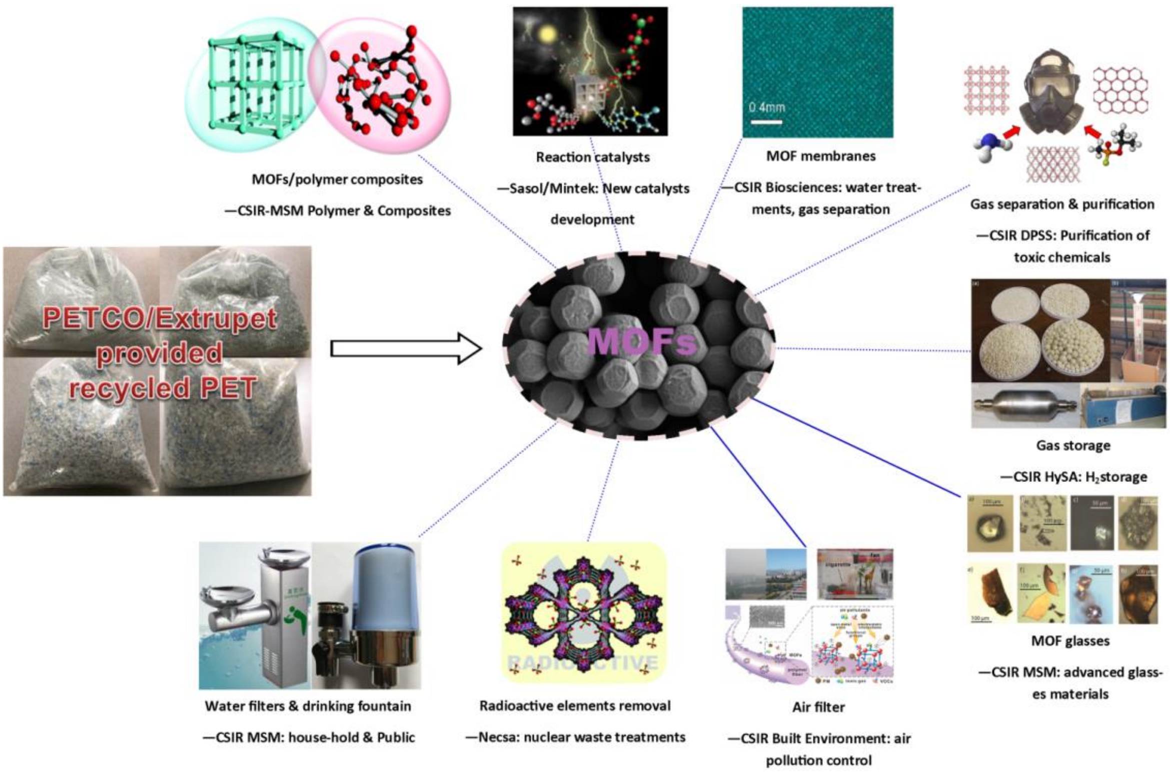


Figure 2: *The immediate interests of MOFs-enabled products at the CSIR*

1.4 Structure of the Report

A literature review on the waste PET to MOFs and the motivation to investigate coloured PET bottles and PET food trays are given in Section 2. The research methodology will be given in Section 3. This covers the KG-scale depolymerisation of coloured PET bottles and PET food trays (Section 3.1), Deduced industrial-scale depolymerisation of coloured PET bottles and PET food trays (Section 3.2), KG-scale of MOFs synthesis (Section 3.3), Deduced industrial-scale MOFs production (Section 3.4), breakdown work packages and key considerations (Section 3.5), evaluation plan (Section 3.6), deliverables (Section 3.7), challenges and constraints (Section 3.8).Section 4 discussed the results and findings from the representative of studying options. This covers the technical feasibility of converting coloured waste PET and food trays to BDC (Section 4.1), Technical feasibility of converting coloured waste PET and food trays-derived BDC to (Section 4.2), Economical appraisal and commercial viability on the business model: converting coloured waste PET and food trays to MOFs (Section 4.3). Section 5 summarizes the outcomes of this project. Section 6 lists the references cited in this report. Annexures (I) attaches the quotation of from Strem Chemicals Inc., and Annexures (I) reports the preliminary technical results towards the feasibility of converting Tetrapak Poly-Alu to MOFs and zeolites.

2. Literature Review

PET as a member of the polyester family of polymers is a condensation polymer produced by the reaction of terephthalic acid (BDC) and ethylene glycol (EG) or dimethyl terephthalate (DMT) and EG. Since the 1960s, PET has been used for the production of many packaging materials for various consumer household goods. The global consumption of PET has been reported to be over 24 million tons per year, and this figure is still increasing annually. 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 and their low efficiencies. Even though the melt-reforming process has been adopted as a route for recycling PET wastes, the obtained products are often of low quality and are limited in their applications. On the other hand, the chemical recycling option is considered as the most ideal recycling strategy because the PET can be depolymerized into its starting monomer or intermediate and can thereafter be re-polymerized.

An emerging and attractive high-value strategy for PET recycling is to use the depolymerized BDC in the production of MOFs. MOFs are a new class of porous materials that 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 commercialization has been due to the high cost of the constituent chemical feedstocks, of which the organic linkers is 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 bring down their cost. In this regard, for the past 6 years, the CSIR has built-up the capabilities to develop different types of MOFs synthesis strategies funded by the DST HySA Infrastructure programme. 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 CSIR research studies had focused on the use of clear PET bottles following a batch synthesis approach. In order to advance the proof of concept and move PET-to-MOF technology towards commercialization, there is a need to investigate the use of other coloured PET bottles and PET food trays, as well as adopt a continuous production method. Importantly, there is also a need to conduct a techno-economic feasibility study on the viability of converting waste PET to MOFs so as to provide the requisite information required for making important decisions for transitioning the research towards the pre-commercialization phase.

In summary, the conversion of waste PET to MOFs has a high potential to contribute to the elimination of waste PET landfilling, minimize overall consumption of crude oil, and retain the chemical value of polyester while generating high-value MOF materials at 40–50% energy consumption in comparison with the use of virgin resin. The completion of this project is hoped that it will create a basis for high-value end-use market for PET-recycling industries. Subsequently, there is potential for creating new industries and job opportunities in the waste sector of South Africa.

3. Methodology

3.1. 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 3a*). Then a solvothermal approach was employed to depolymerize the coloured PET bottles and PET food trays in a 5 L high-pressure reactor as shown in *Figure 3b*. The typical procedure is following:

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

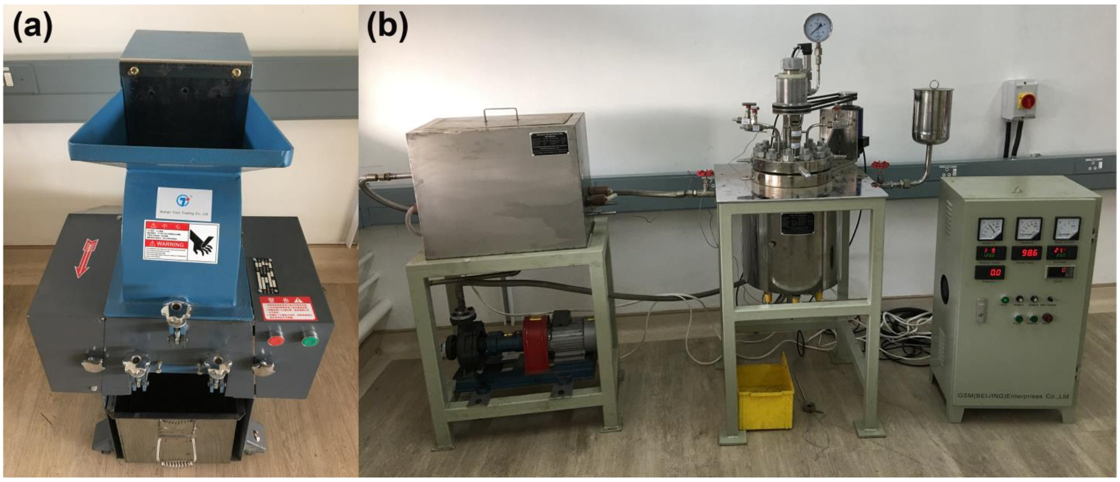


Figure 3: *Digital pictures of: (a) Crusher for PET bottles, and (b) the used 5 L reactor in this project*

The deploymerisation process for the baseline cost assessment is defined in *Figure 4.*

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 4: *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)*

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

Referred to 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 process of the recycled PET raw materials can be combined together with higher energy efficiency, time efficiency and higher automation. The reactor used to depolymerize 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 standardized to take 8 h. The filtration, solvent recycling and vacuum drying steps can be combined together, which has the potential to shorten the total filtration, solvent recycling, washing & drying time from 16 h to 4 h. A comparison of generalized laboratory-scale deploymerisation conditions and our assumed industrial-scale deploymerisation conditions is summarized 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

3.3. 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:

a) The waste PET (coloured PET bottles and PET food trays)-derived BDC and Zr-metal salt were put into the reactor.
b) The calculated amount of DMF was poured into the reactor as a solvent.
c) The calculated amount of formic acid was poured into the reactor as a modulator.
d) MOF UiO-66(Zr) materials were obtained after 8 h at an elevated temperature of 120 °C and an autogenous pressure.
e) The MOF UiO-66(Zr) products were separated from the mother liquid by centrifugation.
f) Products were washed twice in methanol, and dried after being separated from the solvents.

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

The production process for the baseline cost assessment for the representatitve MOF UiO-66(Zr) is defined in *Figure 5.*

3.4. 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 laboratory scale, as described above. However, the laboratory procedures are not well-suited to high production rates based on the engineering judgment, so some variations on the laboratory procedures need also examined as the Industrial Baseline Process. The Process steps, production principles & 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 was transferred directly to scale-appropriate unit operations. This section will describe what assumptions were made to scale-up laboratory-demonstrated synthesis.

At the industrial-scale production, it is assumed that the reaction temperature can be lifted up to 160 °C, so as 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 & 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 generalized laboratory-scale solvothermal reaction conditions and our assumed industrial-scale solvothermal reaction conditions is summarized 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
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.

3.5. Breakdown work packages (WPs) & Key considerations (KCs)

WP 1: Technical feasibility of converting coloured waste PET and food trays to BDC.

KCs: In this WP, a studying case of converting coloured waste PET and food trays to BDC in a 5 L reactor was chosen, and properties of the obtained BDC were compared with commercial feedstocks.

WP 2: Technical feasibility of converting coloured waste PET and food trays-derived BDC to MOF UiO-66(Zr).

KCs: In this WP, a studying case of converting coloured waste PET and food trays-derived BDC to MOF UiO-66(Zr) in a 5 L reactor was chosen, and properties of the obtained MOF UiO-66(Zr) were compared with those obtained from commercial feedstocks.

WP 3: Economical appraisal of converting coloured waste PET and food trays to 1 kg MOF UiO-66(Zr) in a 5 L reactor.

KCs: Following the WP1 and WP2, the process-based cost estimation methodology was used to assess the production cost of the representative MOF UiO-66(Zr). In this step, the actual steps of MOF UiO-66(Zr) production was followed to determine the final cost by summing up the individual costs incurred in each step of the process. The detailed description of the approach can be found below.

For each identified step in the production process, a cost is tabulated based on the materials used in that step, the cost of the capital equipment for the step, and the machine and labor operational time to complete each step. Price quotes for each of the chemical reagents and necessary capital equipment are collected from the suppliers. Operational time calculations are determined from detailed mass and energy balances including reaction kinetics and yield for the system along with product information on equipment and reaction cycling times, and standard operating procedure for chemical operations. The CSIR standard labor and manufacturing rates, as well as utility prices are used to determine the final production cost of the MOF products.

WP 4: Commercial viability of converting coloured waste PET and food trays to MOF UiO-66(Zr).

KCs: Following the WP1, WP2 and WP3, the commercial viability of the business model of converting coloured waste PET and food trays to MOF UiO-66(Zr) was evaluated. Costs were assessed at a production rate of 10KG/day of BDC and Zr-MOF. For the projected Zr-MOF, cost correlates to a production facility optimized for that level of production: MOF UiO-66(Zr) costs are not merely that costs from a large facility operated at lower than design capacity.

For standardized materials and devices, price quotations from industry as a function of annual order quantity form the basis for financial estimates. A learning curve formula is then applied to the available data gathered from industry to provide price estimates between the quotation data points.

When nonstandard materials and devices are needed, costs are estimated based on detailed DFMA style models developed for a specific, fully defined, manufacturing process train. In this approach, the estimated capital cost, C_{Est}, of a manufactured device is quantified as the sum of materials costs, C_{Mat}, and the manufacturing costs, C_{Man}. Given that, in a chemical process, no tooling or assembly is usually required, there costs are not considered in the technical economic analysis, However, a contingency cost was added, which increases the manufacturing cost by 10%:

$$C_{Est} = C_{Mat} + C_{Man}$$

The material cost is derived from the number of raw materials needed to make each intermediate or chemical product, based on the system physical design.

WP 5: Risk assessment of converting of coloured waste PET and food trays to MOF UiO-66(Zr).

KCs: By taking into the overall process into consideration, the following can be identified as the main risk factors: (1) The usage of toxic DMF as a solvent and formic acid as modulator can pollute the workplace and can be the risk to the health of the operators. (2) The highly required expertise in MOF materials science and manufacturing can be a factor that determines the chances of success or failure of the MOF production process. Therefore, the control measures need to be in place to secure the success of the MOFs manufacturing process.

3.6. Evaluation plan

Project evaluation will be the responsibility of the project evaluator and consist of two different evaluative strategies- lab experiment and practical application. An annual report will be issued that presents the evaluative findings.

3.7. Deliverables

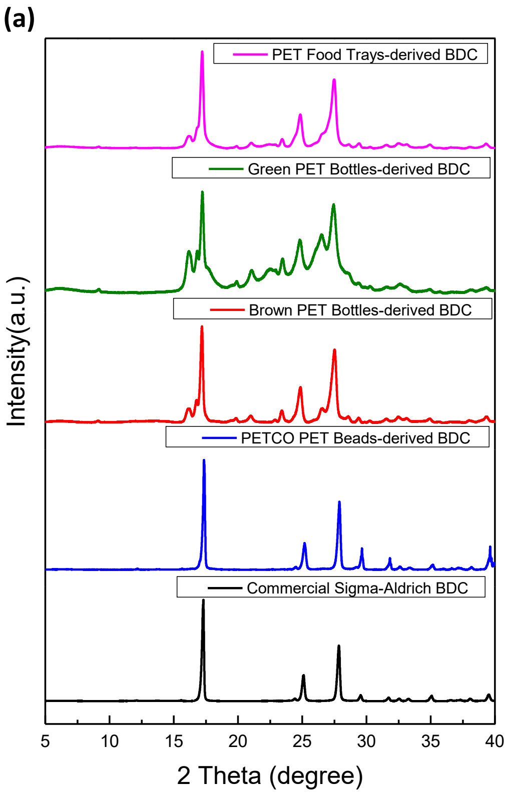
By the completion of this project, technical feasibility and a techno-economic evaluation report on the proposed business model of waste PET-to-MOFs will be submitted back to DST/PETCO. The report will cover the outcomes of the technical viability for the use of coloured PET food trays and bottles, economical appraisal and risk assessment of producing MOFs from coloured waste PET and food trays. In addition, the recommendations will be made for further actions towards the proposed technology.

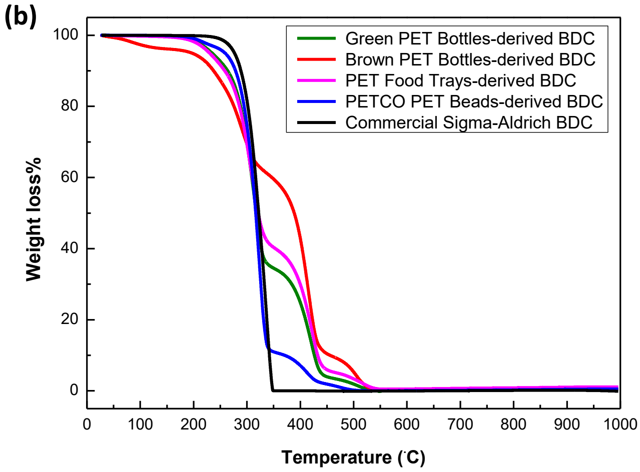
3.8. Challenges and Constraints

There were a number of challenges associated with this work such as the delay of chemicals delivery, the requirement of highly technical expertise on different BDC-based MOFs materials, engineering knowledge towards the scaling-up of MOFs production to KG-scale, the availability of economist and handling of hazardous solvents.

4. Results and Findings

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





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 6**: (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*

Figure 6a shows the X-ray diffraction (XRD) patterns of the BDC products from different PET sources. As 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 6b* that the purities of the different BDC samples are slightly different.

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

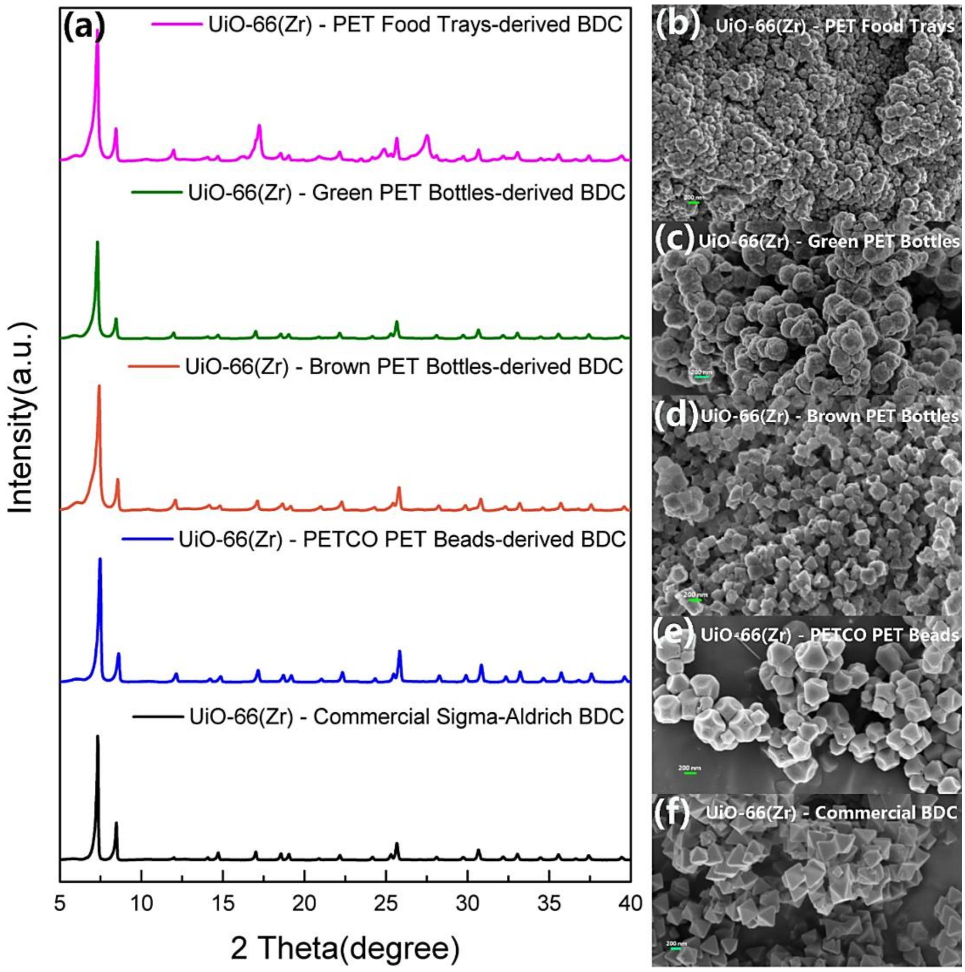


Figure 7: *(a) XRD patterns, and (b-f) SEM images of the Zr-MOF samples prepared from different BDC sources*

Several characteristic reflection signals in *Figure 7a* 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 synthesized from Green PET Bottles-derived BDC shows the lowest relative crystallinity. The scanning electron microscope (SEM) images in Figure 7b-f show the quite differed morphologies of the obtained MOF UiO-66(Zr) samples.

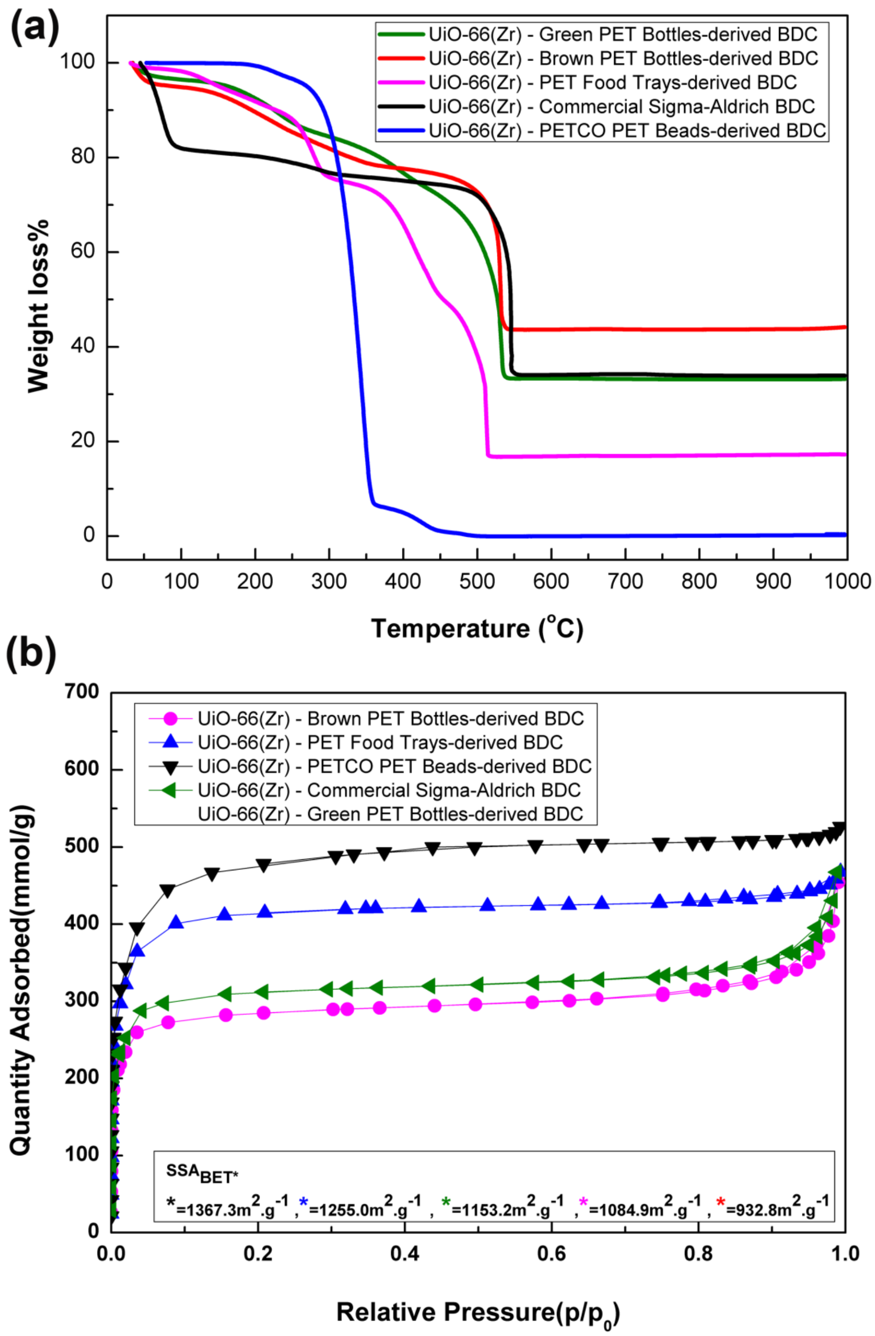


Figure 8: *(a) TGA curves and (b) N_2 sorption of the MOF UiO-66(Zr) samples prepared from different BDC sources. Right bottom Table: BET and H2uptake results of the prepared MOF UiO-66(Zr) samples*

Figure 8a 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 8b* and *8c* 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 in the bottom of Figure 8b) 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 synthesized from the coloured PET bottles-derived BDC, where the effects of additives and colourants should be taken 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 the lower textural properties than those from the clear PET beads-derived BDC. The reason could be the effects of additives and colourants from the green and brown coloured bottles.

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

4.3.1. Costing factors and assumptions in KG-scale

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

Cost calculations of KG-scale depolymerisation of coloured bottles & 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	E.G.	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

Cost results of KG-scale depolymerisation of coloured bottles & 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 amortized over equipment lifetime as well as process energy, utilities, labor and facility costs. As seen, the machinery costs dominate the total costs for the KG-scale depolymerisation of coloured bottles & PET food trays to produce BDC. Apparently, the profitability of this case is very low, and there is the potential to lower the manufacturing costs by scaling-up the process.

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

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.

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.

Cost results of KG-scale MOF UiO-66(Zr) production from waste PET-derived BDC trays are presented in *Table 4*. 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 (date: 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 hours (based on an hourly rate of a salary of R500k annually) for three technicians requested. As the price of is not available from the Sigma-Aldrich website, a levelized 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 of raw materials (salts, linkers, and solvents), while manufacturing costs reflect the cost of machinery amortized over equipment lifetime as well as process energy, utilities, labor 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.

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.

4.3.2. Costing factors and assumptions in 10KG-scale

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

Cost calculations of 10KG-scale depolymerisation of coloured bottles & 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 H_2O	100	-	82	**182**
Depolymerisation 8 h/batch	50L reactor	500,000	E.G.	368	14	1308	**501893**
			D.I H_2O	100	103		
Filtration & Washing, 3.5 h/batch	Presser	68,000	Filtration	50	1	573	**68724**
			D.I H_2O	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 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 anymore in the laboratory. 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 Marketing & Sales, Technician and Accountant with annual salary packages of R310399, R261641, and R282413, respectively.

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

Cost calculations of 10KG-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	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**

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. When coming to the industrial-scale operation, three employees will be hired including Marketing & Sales, Technician and Accountant with annual salary packages of R310399, R261641, and R282413, respectively.

4.3.3. Financial Viability

The theory of financial viability measure to outputs, namely;

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

A sound investment means an ability to generate 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 success 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 the prospective investors, encouraging them to contribute equity funds to the particular project rather than to employ them elsewhere. Contributing equity investments into 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 decision are based on 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	2019e	2020e	2021e	2022e	2023e	2024e	2025e	2026e	2027e	2028e	2029e
Index	0	1	2	3	4	5	6	7	8	9	10
Subsidies	0										
Equity	130 439										
Private Withdrawal											
Loan	521 755										
Total Investment Payout	(652 194)										
CASH POSITION	**(236 400)**	**1 286 315**	**998 916**	**1 051 063**	**1 106 213**	**1 165 277**	**1 229 912**	**1 303 203**	**1 391 078**	**1 505 309**	**1 670 124**
Cash Position cumulated; negative values compensated by current account	(236 400)	1 049 915	2 048 831	3 099 895	4 206 108	5 371 385	6 601 297	7 904 500	9 295 578	10 800 887	12 471 012
Cash Flow after Dept Service, after tax	(236 400)	1 286 315	998 916	1 051 063	1 106 213	1 165 277	1 229 912	1 303 203	1 391 078	1 505 309	1 670 124
Cash Flow after Dept Service, before tax	(236 400)	1 641 502	1 373 085	1 445 148	1 521 316	1 602 803	1 691 814	1 792 452	1 912 590	2 067 839	2 308 548
Equity	(130 439)										
Free Cash-Flow (before tax) to Equity	(366 839)	1 641 502	1 373 085	1 445 148	1 521 316	1 602 803	1 691 814	1 792 452	1 912 590	2 067 839	2 308 548

Table 9: *IRR and NPV to equity*

IRR to EQUITY											
4.35%											
Free Cash-Flow to Equity	(366 839)	1 641 502	1 373 085	1 445 148	1 521 316	1 602 803	1 691 814	1 792 452	1 912 590	2 067 839	2 308 548
Benchmark Discounting after 2019	1.00	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	(366 839)	1 492 275	1 134 781	1 085 761	1 039 079	995 215	954 985	919 811	892 237	876 966	890 045
NPV to EQUITY											
(R 20 082.31)											
Auxiliary Calculation/ Loan											
Debt as at 01.01.	521 755	474 323	426 891	379 458	332 026	284 594	237 161	189 729	142 297	94 865	47 432
Debt as at 31.12.	474 323	426 891	379 458	332 026	284 594	237 161	189 729	142 297	94 865	47 432	0
Interests as at 31.12	52 176	47 432	42 689	37 946	33 203	28 459	23 716	18 973	14 230	9 486	4 743
Repayment as at 31.12.	47 432	47 432	47 432	47 432	47 432	47 432	47 432	47 432	47 432	47 432	47 432
Auxiliary Calculation/ Depreciation											
Investment/ years	0	0	0	0	0	0	0	0	0	0	0
Investment/ 10 years	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	
Replacement Investment/ 5 years	0	0	0	0	0	0	0	0	0	0	0
Total	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	(65 219)	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 tax of the project is greater than the cost of capital, it can be concluded that the project is financially viable. The production machinery that manufactures products is to recover funds and the terms of repayment loans need 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 the 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%**.

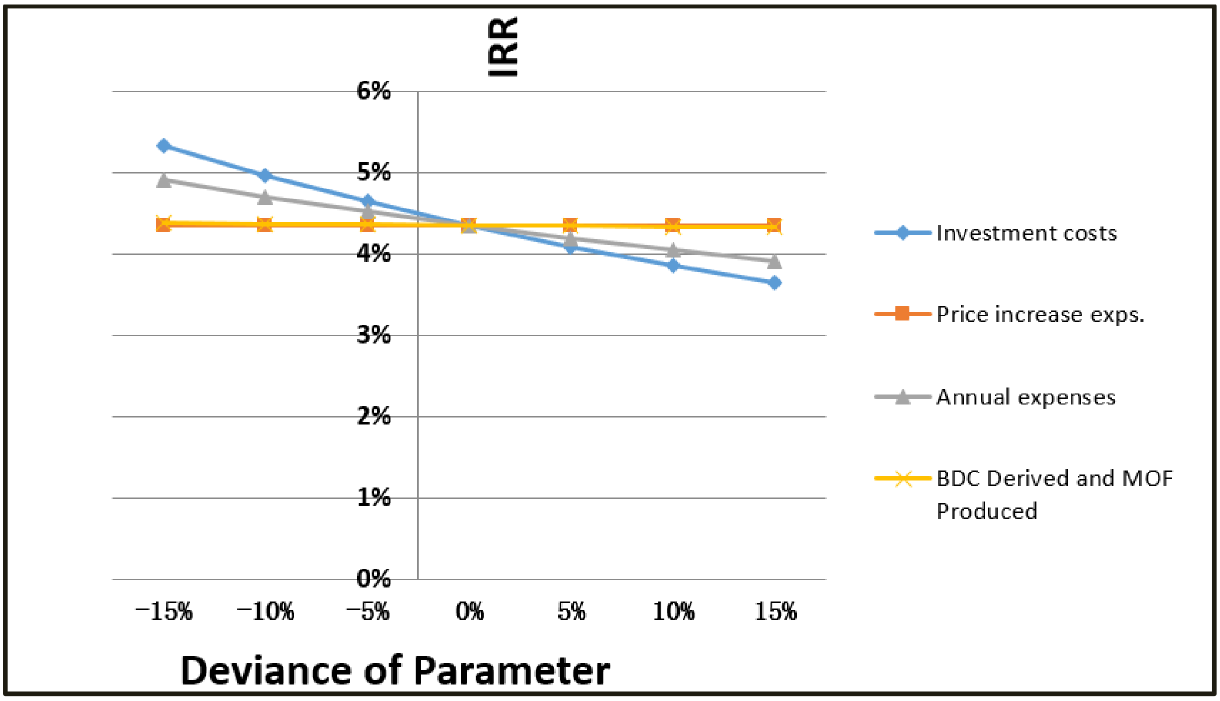


Figure 9: *Estimated internal rate of return*

Figure 9 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 of over-capitalisation 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 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 mobilized by reinvesting back profits.
Certain factors need to be considered when external financing is considered. These include among others, 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 risks faced any plant has an important bearing on the type of financing that should be used. The greater the business risk, the less desirable debt financing usually becomes relative to equity financing. Equity financing is safer in that there is no contractual obligation to pay interest and repay principal as there is with a loan.

4.3.4. The financial and economic analysis

There are two ways that 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 analysis, 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 financially 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 Financial analysis for a project plant that would produce MOFs have been considered. This means that the cost that would have been spent on landfilling PET waste has not been measure calculated as well as potential incomes stream for climate change mitigation.

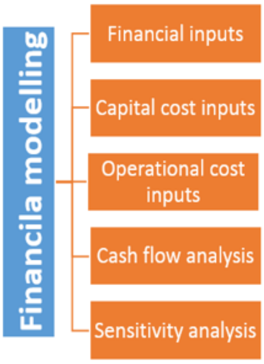
4.3.5. MOFs financial modelling results

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 calculation for the infrastructure energy and water usage have been estimates using utility tariffs respectively. The estimation of capital investment cost has comprised 7 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 10*. 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 10: *Modelling input and results*

The calculated financial results from data shown in *Figure 11* are based on a yearly production of MOFs and the derived BDC that generate 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.

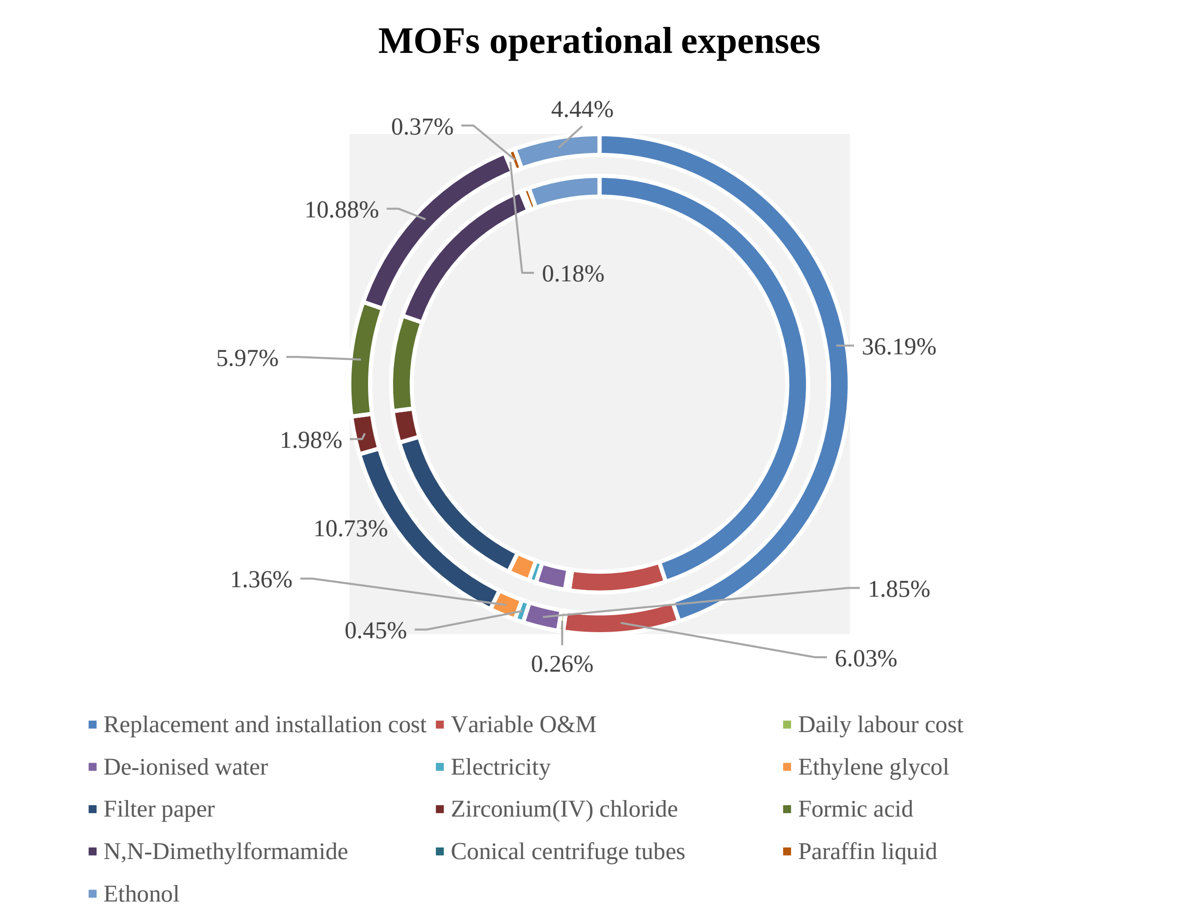


Figure 11: *MOFs operational expenses*

Depreciation has been 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 12*. 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 12*.

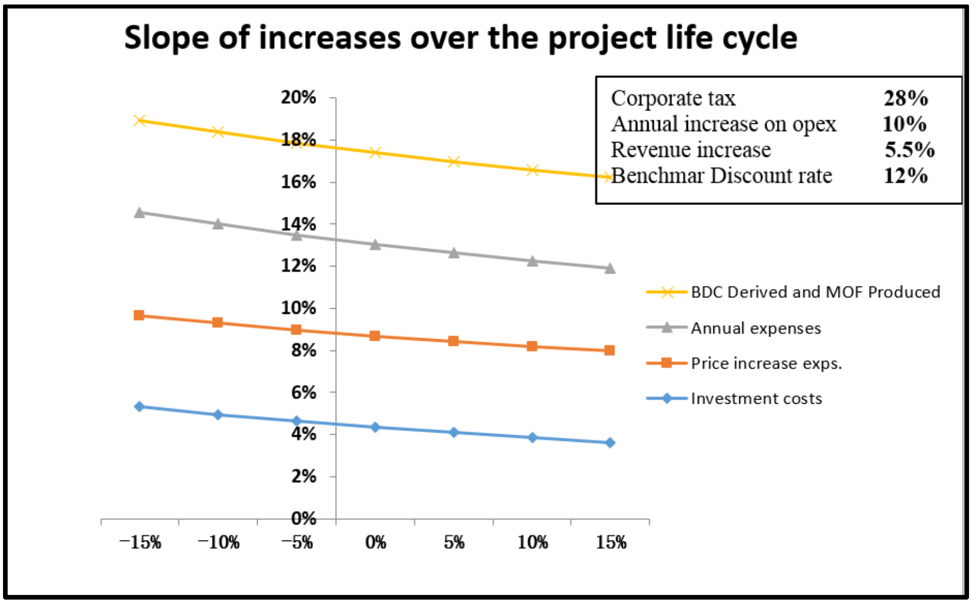


Figure 12: *Project costs escalation rate slopes*

4.3.6. 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.

4.4. 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, i.e. highly technical expertise on MOFs materials	Employ technical expertise
High set-up costs for a MOF producing facility	Partnership with other industries
Engineering knowledge towards the scaling-up of MOFs production	Involved quality chemical engineers
Usage of organic solvents i.e. 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 under compliance with national/international standards. There are no other clearances and objection certificates required.

5. 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 technically proved feasible. The production costs can be significantly reduced at an industrially relevant scale. Given the different BDC-based MOFs, the selection of manufacturing method will be determined by which method fits best with a particular MOF, and it is recognized that a fully continuous synthesis operation has 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%) is 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 minimize solvent usage are also recommended. Similarly, reduction of material cost and size of reactors could also contribute in reduction of MOF manufacturing cost.

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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ANNEXURE 1

TITLE –Quotation from Strem Chemicals Inc. on

>>> Cory Richford <crichford@strem.com> 28/03/2019 18:15 >>>
Hello,

We can offer the following for 1000g of our 40-1105 material.
If partial shipments are something that you would prefer we can confirm details at the time of order.

Customer:	For: CSIR Re: Quote# 47281			
Contact Name:	For: Xoliswa Dyosiba Quoted by: Cory and CC/JB			
Strem Item:	40-1105 Zirconium 1,4-dicarboxybenzene MOF (UiO-66) [1072413-89-8]			
Quantity @ Price	**Total**	**Quoted as: Quant x Size**	**Shipment**	**Price/Pack**
1000 g @ $20/g	$20000	1 x 1000 g	6-10 Weeks ARO, partial shipments are possible	$20000/1000g
Note:	Net Value. Freight is additional charge! Confirm price at time of order! Payment terms to be negotiated.			

The terms are FCA Newburyport, Massachusetts and net 30 days. All sales are made subject to Strem Chemicals, Inc. Terms and Conditions of Sale available upon request or at "http://www.strem.com". This quotation is valid for 30 days, but we reserve the right to make price changes at any time. Prices quoted do not include special packaging requirements necessary for shipping. Leadtime is dependent upon stock availability at the time of order placement. This quote is for this quantity only. Orders placed for lesser or greater quantities must be requoted. Please contact our customer service representatives (cc list) if you have any questions or would like to place an order.

Best Regards,
Cory

Cory Richford | *Customer Service Specialist*
Strem Chemicals, Inc., an employee-owned company
7 Mulliken Way · Newburyport, MA · 01950-4098 · USA · **www.strem.com**
Email: crichford@strem.com · Tel: 978-499-1670 · Fax: 978-465-3104
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We welcome your comments and suggestions.

ANNEXURE 2

TITLE –Preliminary technical results towards the feasibility of converting Tetrapak Poly-Alu to MOFs and zeolites

Background

Recycling of polymer-based multilayer packaging materials presents an ongoing challenge worldwide. The common multi-layered materials that are often referred to as 'Tetra Pak' postconsumer packaging materials are the most widely used packaging materials for perishable food products such as juices and dairy products due to their ability extended their shelf life. Conventionally, Tetra Pak packaging materials are produced through the process of laminating a paper board, Low density Poly Ethylene (LDPE) and a thin Aluminium foil (Al) in order to form a layered composite material. The composition of the Tetra Packages are typically composed of 75% of Paper, 20% LDPE and 5% Al foil and each of this layer serving an important role for food preservation. For example, the paper board aims to improve on the materials strength, Al foil serves to provide protection from light, odours, microorganisms (among others) whereas the polymeric layer (mostly LDPE) aims to protects the food content from getting in direct contacts with the aluminium layer as well as acting as a bonding material during the hot sealing process. Due the complexity of this layered structure, these materials often present a challenge during the recycling stage. Therefore, the significant accumulation of the used Tetra Pak type packaging material in the waste dumps requires dedicated innovative technologies that will not only make the recycling technology economically feasible but also ensure sustainability of the recycling process. Broadly, the common practices for recycling tetra pack can be classified into two main categories i.e. 1) those relying on hydropulping as the first step to enable the separation of the cellulosic fibre from Poly-Al laminate, and 2) those based on recycling the whole packaging material as it is. The approach of non-separated recycling often involves energy recovery (either facilitated by incineration, gasification or pyrolysis) or by reforming/processing them to obtain low quality products such as laminated boards or other shaped products through hot-pressing with other binders. On the other hand, the process involving hydropulping approach typically results in a paper pulp that is processed into different paper-based products and Poly-Al laminate/composite.

State-of-the-art for recycling rejected Poly-Al composite

The Poly-Al composite resulting from the hydropulping-based Tetra Pak recycling is typically composed of 20% Al and 80% Polyethylene. Technologies for optimal and high value recycling of the Poly-Al are still under development. In most cases, the Poly-Al composite is mainly used for energy recovery either through direct incineration or through pyrolysis. The solid materials obtained from the energy recovery route are often of low value since they are mostly either Al2O3 or a mixture of Al and Al2O3. Alternatively, the Poly-Al composite can also be shaped into other functional materials through hot-pressing or moulding to result in items such as roof-tiles, trays, among others. There are still other studies that have reported on either acid or solvent-based delamination approach to recover Al and LDPE powder. Additionally, there are reports on application of a solvent based extraction process for recovering LDPE by dissolving it in an organic solvent at elevated temperatures followed by separation of undissolved materials (Al and/or residual paper or other polymers). Owing to the fact that the existing technologies for recycling Poly-Al composite are either too complicated or often results to low-value products that makes their recycling unattractive, there is a need to develop other approaches or technologies that can contribute in making the recycling of the Tetra Pak-based packaging more economically feasible and meanwhile, obtaining high value-added products.

About the developed invention

The invention developed in this study discloses a process for recycling the hydropulping-derived Poly-Alu composite (or even untreated Tetra Pak packaging materials) to generate high value chemical feedstocks such as; sodium aluminate, aluminium hydroxide and aluminium suphate, among others. The obtained chemicals can be used as recovered or can further be utilised in the synthesis of high-value porous materials such as zeolites and metal-organic frameworks (MOFs) that are known to have a wide range of applications. The approach reported in this disclosure introduces the aspect of incorporating metal or non-metal hydroxides, carbonates, chlorides, sulphates etc. either during the direct incineration or pyrolysis process in order to generate Al-based reactive chemicals such as sodium aluminate that can be used for zeolites synthesis. Additionally, others derivatives such as aluminium sulphate (Al2(SO3)) can be used in applications such as water treatment or even as a feedstock for the production of Al-based Metal organic Frameworks (MOFs) through additional of an organic linker in pre-determined reaction conditions.

Details for the filled provisional patent are as below;

Title of invention: Recycling or processing of layered packaging materials.

COPY OF PROVISIONAL SPECIFICATION

Application No.	2018/07422
Filing Date	6 November 2018
Your Ref	
Our Ref	P82485ZP00
Name of Applicant(s)	CSIR
Name of Inventor(s)	MUSYOKA, Nicholas REN, Jianwei
Title of Invention	RECYCLING OR PROCESSING OF LAYERED PACKAGING MATERIALS
Completion Date	6 November 2019

The specification has been drafted and the patent application has been filed on the assumption that the invention is "new". The fact that we have undertaken to file this application should NOT be interpreted as an indication or guarantee that a valid patent will be obtained for the invention.

If a patent based on this application is granted then its term will be 20 years commencing with the date of filing of the complete specification, subject to payment of renewal fees.

Please keep us promptly advised of any change of contact details.

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