MOFs industrialization: a complete assessment of production costs

Maria Inês Severino[a, b], Effrosyni Gkaniatsou[a], Farid Nouar[a], Moisés L. Pinto[b], Christian Serre[a]

[a.]Institut des Matériaux Poreux de Paris (IMAP), UMR 8004 CNRS, Ecole Normale Supérieure de Paris, Ecole Supérieure de Physique et de Chimie Industrielles de Paris, PSL Research University, 75005 Paris, France

[b.]CERENA, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

1. Characterization

X-Ray Powder Diffraction

Data was collected on a high throughput PANalytical Empyrean diffractometer with CuKα radiation (λ=1.5418 Å) and equipped with a PIXcel 1D detector.

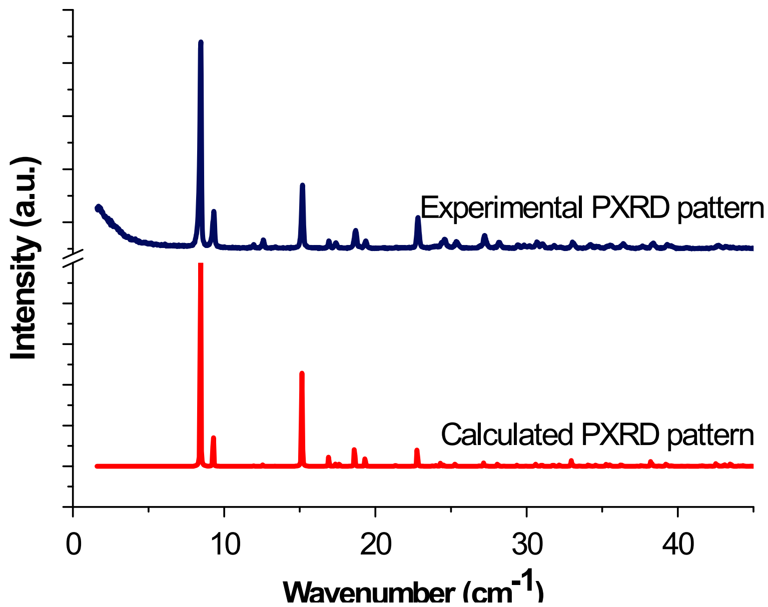

Fig. S1. X-ray powder diffraction (PXRD) for MIL-160(Al) synthesized with the 30 L pilot scale reactor (blue) compared to the calculated (red) in 2 Ɵrange from 1.6 to 45 □.

Nitrogen Sorption

The Nitrogen (air liquid, 99.999%) sorption isotherm was measured at 77 K using a liquid nitrogen cryogenic bath, Micromeritics Tristar instrument. Prior to the analysis, the sample was degassed at 473 K for 5 hours. The obtained accessible surface area was 1130 $m^2 \cdot g^{-1}$ for MIL-160(Al) produced in the pilot 30 L reactors, and the pore volume was about 0.40 $cm^3.g^{-1}$, in agreement with the values published for MIL-160(Al) produced in a 2 L scale (calculated using the BET model)[1].

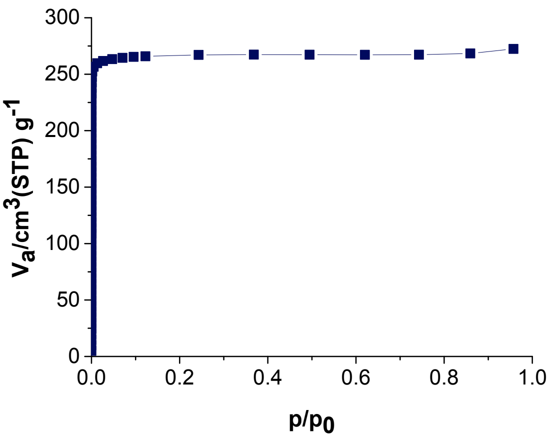

Fig. S2. Nitrogen sorption isotherm for MIL-160(Al) synthesized in a 30 L pilot-scale reactor.

Thermogravimetric Analysis (TGA)

Thermogravimetric analysis was performed using a Mettler Toledo TGA/DSC 2, STAR system apparatus with a heating rate of 5 °C/min (Oxygen flow). The weigh losses are in good agreement with the expected range; about 74 % ligand loss for MIL-160(Al) (72 % calc.).

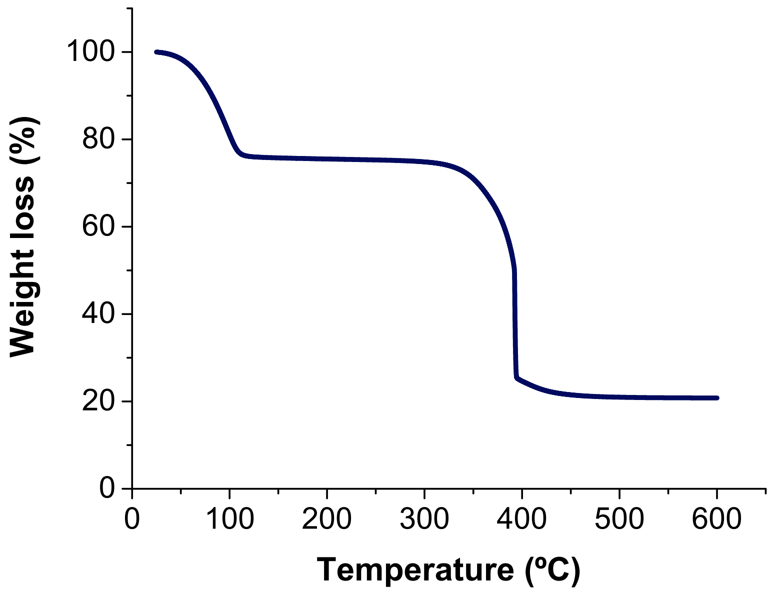

Fig. S3. Thermogravimetric analysis profile for MIL-160(Al) under oxygen flow.

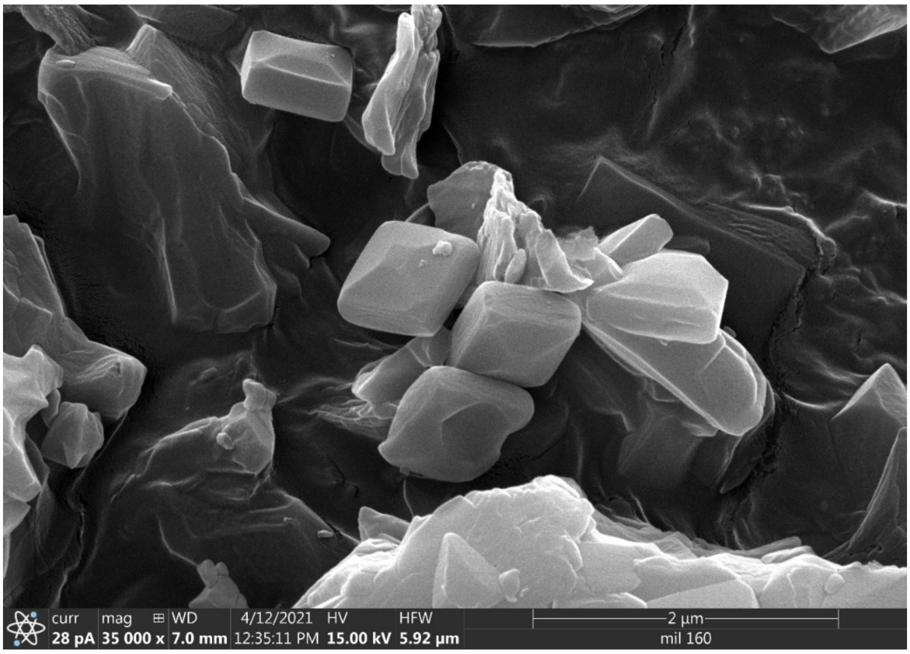

Fig. S4. SEM images of MIL-160(Al) synthesized in a 30 L scale.

2. Production cost estimation calculations:

2.1. Considerations

For the process construction several equipment is required. Reactor, filter and dryer are the main ones. However, accessory equipment choice needs as well to be carefully considered to fulfil the requirements of the process. The choice made are presented in table S1.

Tab. S1 – Different accessory equipment considered in the process to produce MIL-160(Al).

Equipment	Characteristic	Reason of choice
Pumps	Centrifugal	Most commonly used pumps;
Blower	Axial	Positive displacement of air in pneumatic transport
Agitator	Turbine	Low viscosity fluids
	Propeller	
Dust collector	Cyclone	Most commonly used dust collector;

The databases used for the estimation of the equipment cost are not up to date to current prices. All the equipment prices were updated to the 2019 prices using the Chemical Engineering Plant Cost Index, CEPCI.

Tab. S2 – CEPCI values of the years of the data base considered (2002 for MHHE[2] values, 2014 Matche[3]) and the respective project year, 2019.

	CEPCI (2002)	CEPCI (2014)	CEPCI (2019)
CE Index	398.7	576.2	627.9
Equipment	441.8	400.1	764.9
Heat exchangers & tanks	360.8	638	658.8
Process machinery	450.8	673.8	775.4
Process instruments	366.8	410.8	452.5
Pumps & compressors	699.8	938.2	1169.2
Electrical Equipment	340.7	515.3	607.8

The fixed investment is a result of direct and indirect cost values. This is determined by established typical relationships defined in the literature. [4] The chosen relationships are presented in tab. S3 for direct costs and S4 for indirect.

Tab. S3 – Different factors f_2,.. f_9 used in estimation of the direct costs in fixed investment[4].

	Percentage over BE or fixed investment
Assembly of base equipment	0.45
Tubes	0.3
Control	0.3
Buildings	
Land and preparation	
Electronic installations	0.15
Thermal isolation	0.1
Utilities and services ($)	**0.112**
Generated vapor	0.03
Vapor distribution	0.01
Substation electricity	0.013
Electricity distribution	0.01
Water for general use	0.018
Water distribution	0.008
Air of instrument	0.01
Treating effluents	0.013

Tab. S4 – Different factors f_1', f_2' and f'' used in estimation of the indirect costs in fixed investment.

	Percentage over direct cost
Project cost and control	30%
Buildings cost	30%
Provision for unforeseen events	15%

Tab S5 – Different values obtained for each parcel of the production cost for the two scales considered 1 kton and 100 ton.

	1 kton (M$)	**100 ton (M$)**
Total equipment cost	2.9 M$	1.9 M$
Direct cost	8.8 M$	5.8 M$
Indirect cost	2.9 M$	1.9 M$
Fixed capital investment	14.9 M$	10 M$
	1 kton	**100 ton**
Manufacturing costs	29.5 $/kg MIL-160(Al)	55.2 $/kg MIL-160(Al)
Raw materials	45.8 %	24.5 %
Utilities	12.3 %	12 %
Operating labor and supervision	7.2 %	6.8 %
Maintenance and repairs	2.8 %	9.9 %
Patents and royalties	1.6 %	1.6 %
Operating supplies	0.4 %	1.5 %
Plant overhead costs	9.0 %	13.2 %
Fixed charges (rent, insurance, taxes, deprecitation)	4.4 %	13.8 %
General expenses (total of administrative, distribution, marketing and R&D)	16.6 %	16.6 %

Notes and references

1 A. Permyakova, O. Skrylnyk, E. Courbon and M. Affram, *ChemSusChem Eur.*, 2017, **160**, 1419–1426.

2 M. S. Peters and Klaus D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, McGraw-Hill International editions, 5th edn., 2003, vol. 35.

3 Matches, https://www.matche.com/equipcost/Tank.html, (accessed 1 December 2020).

4 W. R. E. Peters, Max S., Klaus D.Timmerhaus, Equipment cost calculation page - Plant design and economics for chemical engineering, http://www.mhhe.com/engcs/chemical/peters/data/, (accessed 1 December 2020).