Oxygen Separation From Air

1. Motivation

Though O_2 constitutes 21% of air and is ubiquitous, the shortage of oxygen concentrators is acutely felt during this pandemic and has even led to the loss of many lives. The currently established methods for separating oxygen from the air are either by cryogenic distillation or by pressure swing adsorption (PSA).[1] Though cryogenic distillation results in high purity O_2 (<99%), it is highly capital and energy-intensive requiring centralized production centers. Transportation of liquified oxygen is an added challenge. Hence adsorptive and membrane-based separation methods are most suitable for small-scale oxygen concentrators. However, both methods are plagued by serious technological challenges. PSA adsorption relies on the selective adsorption of N_2 on zeolites and is capable of producing O_2 with > 90% purity. However, the presence of even ppm amount of water (humidity) leads to the preferential adsorption of water in zeolites over N_2 leading to a loss of O_2 purity and separation efficiency.[2] In membrane-based separations, similar properties and size of O_2 and N_2, results in very low selectivity from polymeric membranes. In this project, we aim to develop porous polymeric materials with organometallic complexes which promote facilitated transport of one species (O_2) resulting in high separation efficiency. Moreover, these polymers are chemically stable and resistant to water. Since such polymers with organometallic complexes are not explored previously, the feasibility of both adsorptive and membrane-based separation will be investigated.

2. Objectives of the proposal

i. Synthesis and development of porous polymers with organometallic complexes (e.g. cobalt porphyrin) which promotes facilitated transport of O_2 species.
ii. Investigation of gas adsorption characteristics of the developed polymers.
iii. Fabrication of thin, defect-free membranes by spin coating/vacuum filtration techniques
iv. Investigation of gas permeation characteristics of the developed membrane.
v. Exploration of the feasibility of a small scale O_2 concentrator

3. Brief Methodology

3.1. Synthesis and Development of polymers with organometallic complexes

Cobalt containing organometallic complexes such as cobalt porphyrin have a good affinity towards molecular oxygen. It was reported that polymeric membranes contacting cobalt complexes show better O_2/N_2 permselectivity than polymeric membranes alone.[3] However, polymers synthesized from cobalt containing organometallic complexes were never explored for O_2/N_2 permselectivity. We envisage that these polymers would display much higher O_2/N_2 permselectivity owing to the presence of a high density of cobalt complexes. Recent developments in the field of porous organic polymers allow us to synthesize porous polymers using porphyrin and phthalocyanine as building blocks with high surface areas.[4,5] Here we propose the synthesis of various porous organic polymers using cobalt porphyrin, phthalocyanine and salen complexes as building blocks (Figure 1a,b). These polymers are expected to be thermally and chemically stable, and resistant to moisture.

3.2. Fabrication of membranes

The feasibility of three different methods will be investigated for the fabrication of defect-free membranes from porous polymers. The phase inversion method typically leads to asymmetric membrane structure with a thin selective layer resulting in high membrane performance. If a defect-free membrane cannot be made using this approach, the spin coating/dip-coating technique will be explored. The vacuum filtration technique will be a backup strategy to synthesize membranes as it has been successfully employed to synthesize defect-free membranes even from flakes that are of the order of few micrometers in size.

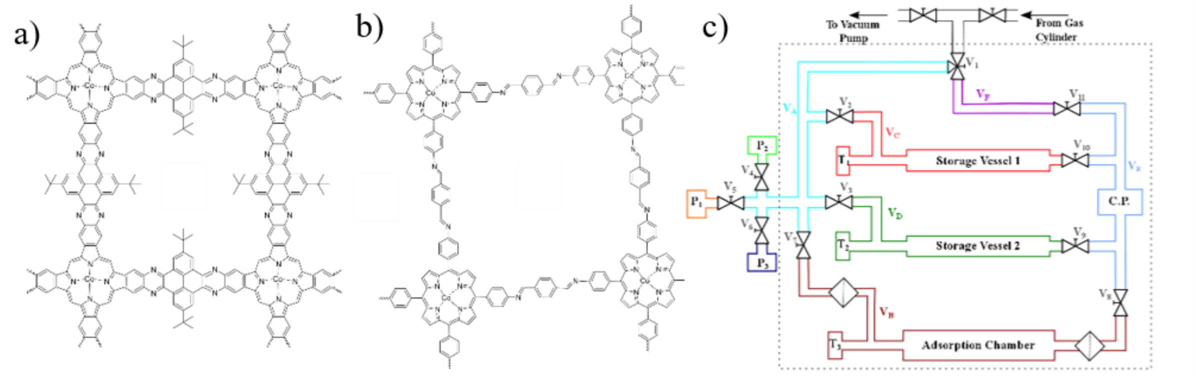

Figure 1. Chemical structures of porous (a) Cobalt phthalocyanine, (b) Cobalt porphyrin (c) Schematic of the proposed volumetric adsorption setup.

3.3. Adsorption and Permeation measurements

A volumetric adsorption setup will be built for studying the adsorption characteristics of the porous polymer (Figure 1c). The proposed setup can measure adsorption properties over a wide range of pressure (0 – 60 bar) and temperature using various gases like O_2, N_2, CO_2 and CH_4. By measuring adsorption isotherms, the isosteric heat of adsorption values can be computed which helps to quantify the interaction mechanism in the adsorbent. The permeation properties of the prepared membranes will be investigated using a self-built permeation setup that can measure the permeation of various gases like O_2, N_2, CH_4 under a range of temperature and pressure. Permeation characteristics will be studied under different temperatures and pressures, and activation energies of various gases will be determined to analyze the mechanism of gas transport.

3.4. Prototype development

Depending upon the adsorptive and permeation properties of the developed porous polymer, the feasibility of developing a small-scale oxygen concentrator will also be explored.

4. Targe population/beneficiaries

Efficient adsorptive/membrane-based O_2 separation is vital for the development of portable O_2 concentrators. The project aims to develop a suitable material for O_2 separation and aims to build a prototype. The portable O_2 concentrator will be useful for medical as well as industrial applications.

5. Expected outcome

The project has both fundamental and technical sides. From a basic science point of view, it is interesting to see how polymers with cobalt-based organometallics aid in oxygen separation. On the practical side, the project aims to develop a novel class of materials for oxygen separation. Hence the project is expected to result in publication in reputed peer-reviewed journals as well as patents. Development of a prototype to demonstrate the feasibility of the proposed method is also part of the proposal.

6. Timeline

Work Schedule (quarters)	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
Synthesis and optimization of polymers with organometallic complexes												

Setting up of adsorption setup	■	■	■	■								
Optimizing membrane fabrication techniques				■	■	■	■	■				
Adsorption and permeation studies					■	■	■	■	■	■	■	■
Prototype development										■	■	■
Publication of results and patents								■	■	■	■	■

7. Budget (in lakhs)

	Year 1	Year 2	Year3
Manpower	3.72	3.72	4.2
Consumables	4	3	3
Adsorption setup and accessories	5	0	0
Prototype development	0	0	5
			Total: 31.64

Proposer Name and Designation

Dr. Deepu J. Babu
Assistant Professor
Materials Science and Metallurgical Engineering
IIT Hyderabad

Dr. Venkata Rao Kotagiri
Assistant Professor
Chemistry
IIT Hyderabad

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