



Ion transport membrane reactors for oxy-combustion – Part I: intermediate-fidelity modeling

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ABSTRACT

Oxy-fuel combustion, particularly using an integrated oxygen ion transport membrane (ITM), is a thermodynamically attractive concept that seeks to mitigate the penalties associated with CO₂ capture from power plants. Oxygen separation in an ITM system consists of many distinct physical processes, ranging from complex electrochemical and thermo-chemical reactions, to conventional heat and mass transfer. The dependence of ITM performance on power cycle operating conditions and system integration schemes must be captured in order to conduct meaningful process flow and optimization studies where multiple degrees of freedom are considered. An axially spatially-distributed, quasi two-dimensional model is developed based on fundamental conservation equations, semi-empirical oxygen transport equations obtained from the literature, and simplified fuel oxidation kinetic mechanisms. Aspects of reactor engineering such as geometric structure, flow configuration and the relationship between oxygen transport, fuel conversion and pressure drop are explored. Emphasis is placed on model robustness, modularity, and low computational expense in order to evaluate the myriad of ITM possibilities within a power cycle simulation quickly and accurately. Overall, the model seeks to bridge the gap between detailed CFD studies and overly-simplified black-box models found in ITM-power cycle analyses, and provides a tool for the analysis and design of ITM systems.

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1. CCS, oxy-combustion and ITM technology

Mankind has reached a critical point in the struggle for secure energy and a clean environment. A plan must be established that will mitigate the harmful effects of increased greenhouse gas emissions and define a framework for alternative forms of power generation to flourish. Currently, thermo-chemical conversion of fossil fuels provides 82% of the global electrical power (roughly 15 TW) and heating requirements [1]. Power generation in particular accounts for 65% of all anthropogenic CO₂ emissions (29 Gt CO₂ in 2007) [1]. Unfortunately, it is unlikely that zero-emissions renewable power generation technology will suffice as a near-term solution due to scaling, energy storage and economic issues among others [2]. Other CO₂ emissions mitigation options include the development of higher efficiency power generation cycles and equipment, the use of less carbon-intensive fuels such as natural gas instead of coal, and carbon capture and sequestration [3]. Anthropogenic greenhouse gas emissions were recently deemed

a “very likely” cause of global warming by a consensus of climatologists and scientists [1], and a sense of urgency has led many to believe that a short term, step-wise reduction in emissions is necessary [2].

This two-part article explores many aspects related to ITM-based power cycles. In part I, an overview of the underlying physical processes required to understand ITM-based power cycles, as well as the complete set of model equations and assumptions required to simulate an ITM air separation unit are provided. In part II, we present case studies that illustrate key performance characteristics, the importance of operational constraints, and suggest design guidelines for the integration of an ITM air separation unit with an oxy-combustion power cycle. Further, we address an important open question in the literature regarding the relative merits of combining oxidation of a fuel with air separation in a single ITM unit. The work herein provides a better understanding of the underlying physics, reveals opportunities to improve the overall ITM system performance, provides the scientific community with a valuable modeling and simulation tool, and allows for meaningful optimization and life cycle analyses to be conducted with greater accuracy than previously available.

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Nomenclature*Latin Letters*

$\bar{C}_{p,j}$	Molar heat capacity at constant pressure of chemical species j [$J \times mol^{-1} \times K^{-1}$]
\bar{h}_j	Molar enthalpy of chemical species j [$J \times mol^{-1}$]
\bar{R}	Universal gas constant 8.314 [$J \times mol^{-1} \times K^{-1}$]
\bar{s}_j	Partial molar entropy of chemical species j [$J \times mol^{-1} \times K^{-1}$]
\bar{U}_i	Overall heat transfer coefficient between streams [$W \times m^{-2} \times K^{-1}$]
\bar{v}_i	Local stream-wise velocity [$m \times s^{-1}$]
$\Delta \bar{h}_{R,k}$	Molar enthalpy of reaction k [$J \times mol^{-1}$]
$\dot{H}_{i,O_2,ext}$	Enthalpy stream of oxygen crossing membrane [W]
\dot{n}_j	Mole flowrate of chemical species j [$mol \times s^{-1}$]
\dot{Q}_i	Convective heat transfer between streams [W]
\dot{S}_{gen}	Entropy generated in ITM system [$W \times K^{-1}$]
ε	Volume void fraction [–]
A	Pre-exponential [$mol \times m^{-2} \times s^{-1} \times Pa^{-n}$]
A_c	Cross-sectional area of one channel [m^2]
A_i	Surface area of a discrete element [m^2]
B	Effective activation energy [K]
Bm_i	Blowing factor [–]
C_V	Oxygen vacancy concentration in membrane lattice [$mol \times m^{-3}$]
D^*	Oxygen ion tracer diffusion coefficient [$m^2 \times s^{-1}$]
D_h	Hydraulic Diameter [m]
D_k	Knudsen diffusion coefficient [$m^2 \times s^{-1}$]
D_V	Oxygen vacancy diffusion coefficient [$m^2 \times s^{-1}$]
D_{ij}	Binary diffusion coefficient of species j [$m^2 \times s^{-1}$]
D_{1m}	Effective binary diffusion coefficient [$m^2 \times s^{-1}$]
F	Faraday constant [$C \ mol^{-1}$]
$F_{i,i+m}$	Overall radiative transfer factor [–]
$f_{i,i+m}$	Geometric view factor [–]
f_i	Local friction factor [–]
Gm_j	Mass transfer conductance of chemical species j [$mol \times m^{-2} \times s^{-1}$]
h^*	Electron hole [–]
J_V	Flux of oxygen vacancies [$mol \times m^{-2} \times s^{-1}$]
J_{CH_4}	Methane flux [$mol \times m^{-2} \times s^{-1}$]
J_{O_2}	Oxygen flux [$mol \times m^{-2} \times s^{-1}$]
k	Mixture thermal conductivity [$W \times m^{-1} \times K^{-1}$]
k^*	Oxygen ion tracer exchange rate constant [$m \times s^{-1}$]
Kp_k	Equilibrium constant for reaction k [–]
M_{avg}	Average molecular mass [$kg \times kmol^{-1}$]
n	Exponent for flux dependence on partial pressure [–]
$N_{ch,side}$	Total number of channels for a generic stream (e.g. “feed”) [–]
N_{ch}	Number of ITM channels [–]
N_{ele}	Number of discretization points [–]
$Nu_{D_h,i}$	Nusselt number based on the hydraulic diameter [–]
O_o^x	Lattice oxygen [–]
$P_{i,tot}$	Local total pressure [Pa]
P_{O_2}	Oxygen partial pressure [Pa]

Pe_{D_h}	Peclet number based on the hydraulic diameter [–]
Pr	Prandtl number [–]
R_j''	Local rate of production of chemical species j [$mol \times m^{-3}$]
r_{pore}	Average pore radius [m]
S_{ch}	Monolith channel width [m]
$Sh_{D_h,i}$	Sherwood number based on the hydraulic diameter [–]
St	Stefan Number [–]
t_h	Membrane thickness [m]
$T_{i,M}$	Local membrane temperature [K]
T_i	Local bulk temperature [K]
t_{pore}	Average pore length [m]
V_O^{**}	Oxygen vacancy [–]
$v_{i,k}$	Stoichiometric coefficient of i th species in k th reaction [–]
V_i	Volume of a discrete element i [m^3]
V_{tot}	Total ITM volume [m^3]
X_j	Mole fraction of chemical species j [–]
y	Transverse membrane coordinate axis [–]
$Re_{D_h,i}$	Local Reynolds number based on the hydraulic diameter [–]
CCS	Carbon Capture and Sequestration [–]
ITM	Ion Transport Membrane [–]
$\Delta G_{R,k}^0$	Standard molar Gibbs free energy of reaction k [$J \times mol^{-1}$]
C_{O_2}	Molecular oxygen concentration [$mol \times m^{-3}$]
k_f	Forward surface kinetics exchange rate constant [$m \times Pa^{-0.5} \times s^{-1}$]
k_r	Reverse surface kinetics exchange rate constant [$mol \times m^{-2} \times s^{-1}$]
m_j	Mass fraction of chemical species j [–]

Greek Letters

μ	Mixture viscosity [$kg \times m^{-1} \times s^{-1}$]
μ_v	Oxygen vacancy chemical potential [$J \times mol^{-1}$]
ϕ	Fraction of total ITM volume allotted to the feed stream [–]
Φ_{jk}	Wilke’s mixture rule constant for species j in species k [–]
ρ_i	Local density [$kg \times m^{-3}$]
τ	Tortuosity [–]
ξ_k	Extent of the k th reaction [$mol \times s^{-1}$]
σ_V	Oxygen ion conductivity [$s \times m^{-1}$]

Superscripts

'	Property of “feed” or oxygen rich stream [–]
''	Property of “permeate” or oxygen deficient stream [–]

Subscripts

e	Property in the free stream [–]
i	Index of a discrete element [–]
j	Index of chemical species [–]
k	Index of chemical reaction [–]
m	Number of discrete volume elements away [–]
o	Property at the surface [–]

1.1. Conventional CCS

Carbon capture and sequestration (CCS) allows for the continued use of fossil fuels without the associated CO₂ emissions and provides an opportunity for a transition to renewable sources of energy. Broadly, CCS entails some sort of gas separation process

resulting in a high-purity CO₂ product stream compressed to high pressure, typically to a supercritical state [3], for storage. There are many methods available to separate CO₂, each with a different engineering approach, underlying physical processes, cost, practicality and thermodynamic penalty [2]. Current First Law efficiencies for CCS power cycles are typically on the order of 35% [2],

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