Applied Thermal Engineering 112 (2017) 378–391

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

Numerical investigation of liquid methanol evaporation and oxy-combustion inside a button-cell ITM reactor

Medhat A. Nemitallah [a,b,*], Mohamed A. Habib [a]

[a] KACST TIC on CCS and Mechanical Engineering Department, KFUPM, Dhahran 31261, Saudi Arabia
[b] Department of Mechanical Engineering, Faculty of Engineering, Alexandria University, Alexandria 21544, Egypt

HIGHLIGHTS

- Analysis of liquid methanol evaporation and oxy-combustion in an ITM reactor.
- A semi-empirical model is applied after fitting with the available LNO membrane data.
- Influences of inlet fuel fraction, inlet gas temperature and inlet sweep flux are studied.
- High combustion efficiency is encountered at moderate inlet gas temperatures.
- High fuel concentration at low inlet sweep flow resulted in high oxygen flux.

ARTICLE INFO

Article history:
Received 15 February 2016
Revised 13 August 2016
Accepted 10 October 2016
Available online 12 October 2016

Keywords:
CFD modeling
Liquid fuel evaporation
ITM reactor
Oxygen permeation
Oxy-combustion

ABSTRACT

A numerical study is conducted to investigate the performance of a button-cell LNO-ITM reactor utilizing the soot-free oxygenated liquid methanol under oxy-combustion condition. The Euler-Lagrange approach is utilized to solve discrete phase model. Taylor analogy breakup (TAB) model is used due to its convenience with the cases of low injection speed. A plain orifice atomizer is used for fuel atomization and CO_2 is used as sweep gas. A semi-empirical oxygen permeation model (ABn model) is validated with the available experimental data and is, then, applied in the present model. Over a wide range of inlet fuel concentrations, the results showed increase in oxygen permeation flux of about five times in cases of reacting conditions as compared to the cases of non-reacting cases. The results showed high oxygen permeation flux at low inlet fuel concentrations due to the improvement in the oxygen to fuel ratio toward the stoichiometric conditions. At inlet gas temperatures of 1223 K, 1123 K, 1023 K and 923 K, the combustion temperature approached 1423 K, 1347 K, 1284 K and 1231 K, respectively, indicating an average combustion efficiency of 43% at moderate inlet gas temperatures. High fuel concentration at low inlet sweep flow resulted in high oxygen flux and high combustion temperature.

1. Introduction

For the time being, emission of greenhouse gases, mainly CO_2, is the most critical challenge facing our existence on this globe. By the coming 2050, the emission levels of CO_2 are expected to be increased by about 70% [1]. Most of the new technologies for power generation including renewable energy technologies are not economically visible yet [2]. In the present days, the oil price is reduced to very critical limits at which the developments of new clean technologies are significantly affected. Based on that, the world is forced to use fossil fuels for the production of energy which necessitates the development of technologies that can reduce the emissions of greenhouse gases while burning fossil fuels. Carbon capture (CC) technologies including pre-combustion, oxy-combustion and post combustion carbon capture are considered as the most effective tools regarding the control of CO_2 emissions [3]. Among these carbon capture technologies, oxy-combustion technology is the lowest cost and the most efficient and promising carbon capture technology [4]. This technology can be used in existing power plants with slight modifications and, also, it can be used with the new power plants [5]. As well, oxy-combustion technology does not require any additional chemical separation process for the separation of CO_2. Simply,

* Corresponding author at: KACST TIC on CCS and Mechanical Engineering Department, KFUPM, Dhahran 31261, Saudi Arabia.
E-mail addresses: medhatahmed@kfupm.edu.sa, mahmed@mit.edu (M.A. Nemitallah).

http://dx.doi.org/10.1016/j.applthermaleng.2016.10.069

Nomenclature

2-D	two dimensional	S_i	source/sink term
3-D	three dimensional	*SIMPLE*	semi-implicit method for pressure-linked equations
ABn	oxygen permeation model	*SSE*	sums of the squares of the error
ASU	air separation unit	*TAB*	taylor analogy breakup model
CC	carbon capture	T_M	membrane temperature
CFD	computational fluid dynamics	T_∞	surrounding temperature
CH_3OH	methanol	*UDF*	user defined function
CO	carbon monoxide	*VO*	vegetable oil
CO_2	carbon dioxide	C_P	heat capacity of the particle (J/kg K)
DME	dimethyl ether	m_P	mass of the particle (kg)
DNS	direct numerical simulations	A_p	surface area of the particle (m^2)
DO	discrete ordinates	h	convective heat transfer coefficient (W/m^2 K)
EWBM	exponential wide band model	ε_p	particle emissivity
FB	flow burning	σ	Stefan-Boltzmann constant (5.67×10^{-8} W/m^2 K^4)
HC	hydrocarbons	θ_R	radiation temperature (–)
H_2O	water vapor	d_p	particle diameter (m)
ITM	ion transport membrane	k_∞	thermal conductivity of the continuous phase (W/m K)
ITMR	ion transport membrane reactor	Re_d	Reynolds number based on the particle diameter and the relative velocity (–)
J_{O2}	oxygen permeation flux	*Pr*	Prandtl number of the continuous phase (–)
LES	large eddy simulations	N_v	(kg mol/m^2 s)
LNO	La_2NiO_4 ionic ceramic membrane	k_c	mass transfer coefficient (m/s)
LSCF	lanthanum strontium cobaltite ferrite	$C_{v,D}$	vapor concentration at the droplet surface (kg mol/m^3)
NOx	nitric oxides	$C_{v,\infty}$	vapor concentration in the bulk gas (kg mol/m^3)
PDF	probability density function	m_D	mass of the droplet (kg)
P'_{O2}	oxygen partial pressure in feed side	A_D	surface area of the droplet (m^2)
P''_{O2}	oxygen partial pressure in permeate side	T_D	surface temperature of the droplet (K)
RTE	radiative transfer equation	T_R	radiation temperature (K)
sccm	standard cubic centimeter per minute		

the products of combustion of a hydrocarbon fuel with oxygen consist mainly of CO_2 and H_2O, which can be passed through a simple condenser to separate H_2O and, then, CO_2 is captured [6].

There are two main approaches regarding the application of oxy-combustion technology. The first is through the use of air separation unit (ASU) to separate oxygen from air, and then the produced oxygen is used in combustion in conventional combustion systems. However, this ASU requires additional powering energy for its operation in terms of gas heating (to activate the membrane for oxygen separation) and compression [7]. The second approach is through the use of what's called ion transport membrane reactor (ITMR) technology. In this technology, both oxygen separation and oxy-combustion processes are performed inside the same unit. An ion transport membrane (ITM) is used to separate oxygen from the flowing air in the feed side to the permeate side. In the permeate side, permeated oxygen across the membrane is burned with the provided fuel in a medium of recirculate CO_2 [8]. The resultant design of the ITMR should result in a compact size of the system due to the combination of both the separation unit and the combustion unit in one common unit. Also, the resultant system will not require any additional powering for oxygen separation because the membrane is heated using part of the released heat of combustion.

In the industrial field, the use of liquid fuels is preferred due to many reasons including low volume as compared to gaseous fuels which results in easy handling and transportation and high energy density. This forces the research towards the design of new systems that can handle easily the liquid fuels. However, care should be taken while designing any combustion system utilizing liquid fuel in order to reduce soot formation, reduce NOx emissions, and properly vaporize the fuel [9]. The liquid fuel combustion is utilized in many industrial devices including diesel engines and gas turbine engines. The subject of liquid fuel evaporation and combustion has been studied numerically by Fujita et al. [10] using 2-D direct numerical simulations (DNSs) and by Moin and Apte [11] using large eddy simulations (LESs). Yin [12] performed numerical modeling of *n*-heptane droplets heating and evaporation aiming at the development of a generic model for the conversion of fuel droplet. They were able to develop a computer code for droplet heating and evaporation taking into account droplet dynamics and the interaction between the droplet and the free-stream. Kitano et al. [13] numerically investigated the influence of difference in fuel composition on the droplet evaporation and combustion. They reported that the evaporation rate becomes slower for multicomponent fuel as compared to single fuel. Targeting reduced emission and clean combustion, Jiang et al. [14] experimentally investigated the combustion process of different liquid fuels including diesel, biodiesel and straight vegetable oil (VO) using a novel design flow burning (FB) injector. The measurements of combustion temperature and NOx and CO emissions were recorded in their work. The results showed the capability of the FB injector to produce clean blue flames indicating mainly premixed combustion for all the tested fuels.

Emission control, especially soot formation, is another critical issue in case of liquid fuel combustion. Park and Yoon [15] proposed a two-stage injection strategy for simultaneous reduction of NOx and soot emissions in dimethyl ether (DME) fueled engine. The results showed low NOx, HC, CO and soot emissions while using the pilot injection strategy with advanced main injection. Speth et al. [16] conducted a study on the effect of using alternative jet fuels that are low in aromatic content on the reduction of black carbon emissions from gas turbines. They established a relationship between the reduction in black carbon emissions and the aromatic volume fraction of the alternative fuel. Choi et al. [17] studied the effect of liquid fuel doping on the formation of soot and polycyclic aromatic hydrocarbon in counter flow ethylene