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Numerical study on thermal oxidation of lean coal mine methane in a thermal flow-reversal reactor

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HIGHLIGHTS

- A three-dimensional simulation on thermal oxidation in a TFRR is presented.
- Effects of the main parameters on the reactor behavior are analyzed.
- Symmetrical cyclic operating state is certified.
- The critical self-maintained running conditions are proposed.

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ABSTRACT

This paper presents a three-dimensional numerical investigation on thermal oxidation of lean coal mine methane in a thermal flow-reversal reactor by the finite volume method. The effects of channel length, feed methane concentration, inlet velocity and cycle time on the reactor behavior were analyzed. Results show that the temperature distributions and methane concentration profiles in the reverse-flow semicycle are mirror images of the ones in the forward-flow semicycle. Thus the cycle for the cyclic steady state is symmetrical. The maximum temperature of the reactor rises significantly with the increases of methane concentration and inlet velocity, and it is nearly unchanged with the increases of the channel length and cycle time. Long channel length, high feed methane concentration, low inlet velocity and short cycle time could achieve a wider high temperature zone in the reactor. The minimum feed methane concentration for self-maintained running rises dramatically with the decrease of channel length and the increase of inlet velocity, and it is almost not affected by the change in cycle time. For a desired minimum feed methane concentration of 0.18 vol.% when v_{in} = 1 m/s, the required channel length should not be less than 1.8 m.

1. Introduction

Global warming potential of methane is 20 times higher than that of CO_2, and it is the second biggest contributor to global greenhouse gas emissions. Coal mine methane (CMM) is a general description for ventilation air methane (VAM) (0.1–1 vol.% methane) and gas drained from underground working areas of coal mine. About 64% of methane emissions from underground coal mines are contributed by VAM [1,2]. In 2000, the VAM emission from China was $6.5 \times 10^9\,Nm^3$, meanwhile the value from the worldwide mines was about $16.6 \times 10^9\,Nm^3$ [3]. CMM emissions are estimated to increase to 793 $MtCO_2e$ ($\times$1000 tons CO_2 equivalent) by 2020 [4].

VAM could not be utilized by the traditional oxidation technologies due to its low methane concentration. Hence, an efficient utilization technology for lean coal mine methane becomes a significant challenge. Catalytic flow-reversal reactor (CFRR) and thermal flow-reversal reactor (TFRR) are the two most representative technologies for VAM utilization. The flow-reversal principle is employed by both CFRR and TFRR, which uses a heat storage medium to transfer the heat released by methane reaction to the feed gas [1,4,5]. The only difference between the two technologies is the use of catalyst in CFRR.

Up to now, catalytic combustion of VAM in CFRR has been mostly concerned. Gosiewski [6] performed one-dimensional (1-D) calculations for the methane combustion in a CFRR with heat recovery. It was found that high heat recovery efficiency can be obtained only under high catalyst temperature. Meanwhile high temperature may cause the

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Nomenclature

A_r	the pre-exponential factor, 1/s
c_p	specific heat, J/(kg·K)
$D_{n,m}$	the mass diffusion coefficient for *n*-th species
E_r	activation energy for the reaction, J/mol
$\boldsymbol{e}_y$	unit vector in *y* coordinate
g	gravitational acceleration, g = 9.8 m/s^2
h_n	the specific enthalpy of *n*-th species, J/kg
J_n	diffusion flux of *n*-th species, kg/(m^2·s)
M_g	molar mass of the gas, kg/mol
N	number of chemical species in the system
p	static pressure, Pa
q	total heat flux, W/m^2
R	universal gas constant, J/(mol·K)
$R^0{}_n$	volumetric rate of creation of *n*-th species, kg/(m^3·s)
t	time, s
t_c	cycle time, s
T_g	gas temperature, K
T_s	temperature of the solid, K
$\Delta T_{s\text{-}g}$	temperature difference between solid and gas, K
$\boldsymbol{V}$	velocity vector, m/s
v	velocity, m/s
x, y and *z*	coordinate in *x*, *y* and *z* directions, respectively
Y_{CH4}	the mole fraction of CH_4 species
Y_n	the mole fraction of the *n*-th species

Greek symbols

β_r	temperature exponent
λ	thermal conductivity, W/(m·K)
μ	the molecular viscosity of the gas, kg/(m·s)
ρ	density, kg/m^3
$\boldsymbol{\tau}$	stress tensor
τ_{eff}	effective stress tensor

Subscripts and Superscripts

ave	average
g	gas
in	at the inlet
n	the *n*-th species
r	reaction
s	solid
out	at the outlet
min	minimum
max	maximum

catalyst deactivation due to homogeneous combustion occurring in the gas phase. The experimental results presented by Su and Agnew [7] on VAM catalytic combustion performance showed that space velocity, preheated temperature and the minimum methane concentration were important design parameters of large-scale combustors to fulfill high level of methane conversion. Mei et al. [8] carried out a three-dimensional (3-D) numerical simulation on the catalytic combustion in monolith reactor with modeling the heterogeneous reaction as a single step. The effects of catalyst, temperature, methane concentration and inlet gas velocity on methane conversion were analyzed. Marín et al. [9,10] reported experimental results for the influences of switching time, inlet methane concentration, and gas flow rate on the outlet conversion and stability. Meanwhile 1-D simulations of the performance of different methods for CFRR heat recovery was performed. It was found that extracting gas from the end of the catalytic bed without cooled gas returning is the most stable heat recovery strategy. Wang et al. [3] performed experiments of VAM combustion in a vertical CFRR. The influences of the initial temperature, feed methane concentration, cycle time, and space velocity were tested. A pilot scale CFRR with a central spiral heat exchanger was integrated by Wang et al. [11]. The effects of varying operating parameters including cycle time, methane inlet concentration, and heat transfer flux on temperature fluctuations and temperature profiles were experimentally investigated. Fernández et al. [12,13] demonstrated a bench-scale CFRR with integrated water adsorption. The adsorbent adsorbed water from the inlet gas before reaching the catalyst, capable of eliminating catalyst inhibition, and was regenerated in situ at a higher temperature during the reverse cycles.

Some investigations [14,15] were carried out to compare advantages and drawbacks of TFRR and CFRR. For high VAM concentrations (above 0.4 vol.%), TFRR is proved to be the cheaper and more reliable choice, achieving greenhouse gas mitigation goal and high heat recovery efficiency. Therefore, TFRR is frequently considered to be an attractive option. Recently, many experiments and numerical simulations on the TFRR have been reported. A simple one-step or two-step reaction mechanism model on thermal combustion of methane-air was proposed by Gosiewski et al. [16]. Considerable amounts of carbon monoxide were found experimentally as an intermediate product. Based on the experimental results of kinetic study, Pawlaczyk and Gosiewski [17] proposed a hypothesis that both homogeneous combustion and heterogeneous surface combustion occurred in the gas phase during the combustion process in a monolith bed. The experimental result showed that large specific surface contact with the gas phase could achieve low ignition temperature and small amount of CO in the exhaust gas. Gosiewski et al. [18] performed experiments and 1-D simulations by using two-step oxidation mechanism for a TFRR and confirmed that the temperature distributions of the reactor were not affected by the heat storage capacity of the TFRR wall. Qi et al. [19] carried out 1-D numerical simulations of thermal combustion of lean methane-air mixture in a TFRR by using porous media model and the single-step oxidation mechanism. The effects of inlet velocity and feed methane concentration were investigated. Gosiewski et al. [20] reported experiments and simulation results and revealed that TFRR with central heat exchanger was more tend to thermal asymmetry than the hot gas withdrawal heat recovery structure. Lan and Li [21] simulated the thermodynamic performance in a honeycomb ceramic channel without reaction. The effects of mass flow rate, solid heat capacity, and reversal time on thermal efficiency were investigated. Baris [22] evaluated the applicability of VAM mitigation technologies for an underground coal mine in Turkey. Li et al. [23] introduced a demonstration project for VAM utilization by using TFRR which was conducted in China. The TFRR system could recovery about (31.61–46.82)% energy to generate electricity for itself.

However, the effects of main parameters on the minimum feed methane concentration for self-maintained running, which is an important parameter for equipment design, have not been clearly given in previous research. The effect of channel length on the reactor behavior has not been reported. Moreover, 3-D numerical simulation studies on the thermal oxidation of methane in a TFRR by using two-step oxidation mechanism have been rare. In this paper, a series of 3-D numerical simulation is performed to understand thermodynamic characteristic in a TFRR. The effects of channel length, feed methane concentration, inlet velocity, and cycle time on the reactor behavior are analyzed.