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A control strategy of flow reversal with hot gas withdrawal for heat recovery and its application in mitigation and utilization of ventilation air methane in a reverse flow reactor

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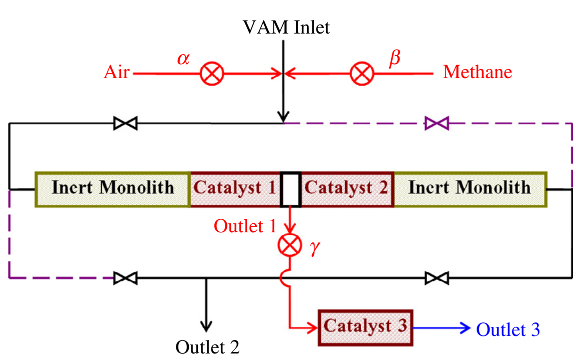
HIGHLIGHTS

- A control strategy was proposed for mitigation of ventilation air methane in a reverse flow reactor.
- Heat recovery and bed temperature regulation are achieved mainly by hot gas withdrawal.
- Air dilution and extra methane injection are used to sustain reaction in some extreme conditions.
- Stability and autothermicity are jointly affected by feed content and hot gas removal fraction.
- High heat recovery efficiency and reactor stability is achieved by using the control strategy.

GRAPHICAL ABSTRACT

A flow reversal control strategy was developed for the mitigation and utilization of ventilation air methane in a reverse flow reactor; heat recovery and bed temperature regulation are achieved mainly by hot gas withdrawal, while air dilution and extra methane injection are the auxiliary variables to sustain the reaction in some extreme circumstances.



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ABSTRACT

A control strategy of flow reversal with hot gas withdrawal for heat recovery was developed and verified for the mitigation and utilization of ventilation air methane (VAM) in a reverse flow reactor. The flow reversal strategy was based on the thermal front propagation velocity and a logic-based controller was built to avoid catalyst deactivation and reaction extinction caused by prolonged rich or lean feed conditions; the utilization of heat released from VAM combustion was considered through heat extraction by withdrawing part of hot gas from the middle of the reactor. By means of simulation using a one-dimensional heterogeneous model, the results revealed that the flow direction should be reversed before the temperature peak passing through the middle of the reactor to reduce the discharge of unreacted methane as well as to enhance the heat recovery efficiency; a fixed (relatively short) switching time is reasonable for the reactor operation in the case of hot gas withdrawal. The stability and autothermicity of reverse flow reactor are jointly influenced by the feed concentration and hot gas withdrawal fraction; the reactor can only be run stably in a narrow operating window (stability area). Heat recovery and

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Nomenclature

a_v	surface area per unit volume ($m^2\ m^{-3}$)
C_{CH_4}	methane concentration (mol m^{-3})
C_P	heat capacity (J kg^{-1} K^{-1})
D	distance of temperature peak movement (m)
Da	Damköhler number
D_{eff}	effective dispersion coefficient ($m^2\ s^{-1}$)
D_R	diameter of reactor (m)
h	heat transfer coefficient (W m^{-2} K^{-1})
ΔH	enthalpy of reaction of methane oxidation (J mol^{-1})
k_m	mass transfer coefficient (m s^{-1})
k	thermal conductivity (W m^{-1} K^{-1})
L	reactor length (m)
P	pressure (Pa)
Pe_H	Peclet number of heat dispersion
Q_{extr}	heat extracted from the reactor (J)
Q_{tot}	heat generated when methane conversion is 100% (J)
$-R_{CH_4}$	rate of methane disappearance (mol m^{-3} s^{-1})
R_g	ideal gas constant (J mol^{-1} K^{-1})
t	time (s)
t_{sw}	switching time (s)
T	temperature (K)
T_α	reference temperature for air dilution (K)
T_β	reference temperature for methane injection (K)
T_γ	reference temperature for hot gas withdrawal (K)
u	superficial gas velocity (m s^{-1})
U_k	overall heat transfer coefficient (W m^{-2} K^{-1})
V_{fr}	front propagation velocity (m s^{-1})
x	axial coordinate (m)
X_{CH_4}	Average methane concentration (mol m^{-3})

Greek letters

α	air dilution term
β	methane injection term
β	dimensionless adiabatic temperature rise
ε	bed void fraction
γ	heat extraction term
γ	dimensionless activation energy
γ_1	fraction of hot gas withdrawal
η	effective factor
η_{th}	heat recovery efficiency
ρ	density (kg tm^{-3})
σ	ratio of volumetric heat capacity of catalyst and gas
τ	tortuosity
Φ	dimensionless temperature increase
ω	dimensionless front propagation velocity

Superscripts and subscripts

0	time $t = 0$
1, 2, 3	bed number
cat	catalyst properties
end	time $t = t_{end}$, the total time of simulation
entr	entrance properties
f	fluid properties
feed	feed properties
in	inlet properties
inj	methane injection
min	minimum value
max	maximum value
out	outlet properties
s	solid properties
sp	set point

bed temperature regulation are achieved mainly by hot gas withdrawal, while air dilution and extra methane injection are the auxiliary manipulated variables to sustain the reaction in some extreme circumstances. An extra catalyst bed along the way to the boiler is effective to enhance the overall methane conversion by oxidizing the unreacted methane. A case study under modified real ventilation conditions shows that the control strategy developed in this work is feasible to mitigate and utilize VAM if the methane content is higher than 0.2 vol.%.

1. Introduction

Coal mining is responsible for 8% of anthropogenic methane emissions and 70% of these emissions come from ventilation air methane (VAM) with a concentration of 0.1–1.0 vol.%, through which a great deal of valuable energy resource was wasted [1,2]. Methane is also the second most significant greenhouse gas after carbon dioxide; since it has a global warming potential of 21 times higher than that of carbon dioxide, combustion of methane that is likely released to air into carbon dioxide is a practicable way to greatly reduce its harmful effect on the climate change [3]. Therefore, the mitigation of VAM emission is of great importance from the view of both energy recovery and environmental protection [4,5].

In comparison with flammable combustion, catalytic combustion can considerably reduce the ignition temperature and thus produces less pollutants; moreover, it allows better control of reaction over a wider fuel/air ratio without concerning the flammability [6–8]. To sustain auto-thermal operation of lean fuel combustion without pre-heating the feed, reverse flow reactor (RFR or FRR) has been proposed to trap heat released by the exothermic reaction. A RFR works under forced unsteady state conditions resulting from periodical switching of the feed flow direction. Owing to the velocity difference between the flowing gas and the temperature front, heat generated by the exothermic reaction can be trapped inside the reactor by selecting an appropriate switching interval, which makes the auto-thermal operation of an RFR possible even under very lean feed conditions. The combination of catalytic oxidation and RFR gives the concept catalytic flow reversal reactor (CFRR or CRFR); in this respect, Matros, Kolios, Zagoruiko et al. have also made some detailed reviews on the mechanism, modeling, applications, history and prospects of this kind of reactors [9–11].

Although a CRFR has numerous advantages such as auto-thermal operation, few harmful emissions, and improved performance than steady-state operation, it is hard to operate due to its hybrid and forced unsteady-state nature as well as the extensive variation of methane concentrations in actuality [10,12,13]. Generally, two