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Parametric study of recuperative VOC oxidation reactor with porous media

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Abstract

Numerical study of volatile organic compounds (VOC) oxidation reactor consisting of two coaxial tubes, filled with inert porous media is performed. Influence of incoming gas flux, adiabatic temperature of gas combustion, reaction rate constant, diameter of porous body particles, reactor size and heat losses on maximal temperature of reactor, recuperation efficiency, combustion front position is investigated. It is shown that maximum temperature and recuperation efficiency of reactor has extremum in the field of incoming gas flow rate and porous body particle size parameters (for simulated configuration of reactor maximum corresponds to $U_G \sim 2$ m/s and $d_0 \sim 6$ mm). Numerical simulation shows non-monotonous character of maximal temperature and recuperation efficiency dependence from side heat losses of reactor. The obtained results can be used for construction optimization of practical VOC oxidation reactors.

Keywords: Filtration combustion (FC); Heat recuperation; Heat regeneration; Porous media; Volatile organic compounds (VOC); Oxidizer

1. Introduction

Air purification from Volatile Organic Compounds (VOC) remains actual problem facing chemical, nutrition, mining and other industries [1,2]. The widely spread VOCs – phenol, formaldehyde, acetone, benzole and other may be contained in ventilation gases of mines, paint shops, plastic extruder shops, in technological flue gases, etc. In many cases VOCs concentration is less than combustion lean limit concentration, but enough for self-sustained combustion in inert porous media. Combustion in inert porous media or filtration combustion (FC) provides effective heat recirculation and consequently low energy costs of the process [3–6]. In the case of sufficiently high concentration of VOCs (~1 mass%) the combustion process may be sustained due to the heat content of the pollutants and does not demand any additional fuels. In experiments by Takeno and Sato [7] in steady reactor with complicated heat recuperation methane–air mixture combustion was realized at equivalence ratio as low as $\Phi = 0.026$ (which is 20 times lower than lean limit combustion concentration for methane–air mixture). In the work [3,4] the regenerative porous media reactor was utilized for lean methane combustion. The stable combustion was achieved at equivalence ratio $\Phi = 0.15$.

One of the principal features of FC is internal heat recirculation in the combustion wave, due to heat exchange between gas and solid in the preheat zone of the combustion wave. Practical systems designed for the low calorific fuels combustion utilize schemes of external heat recirculation in addition to the internal one. These are heat recuperation by means of counter-flow heat exchange between incoming and exhaust gases and heat regeneration due to periodical reverse of flow direction. Both schemes are investigated in laboratory installations [3,4,8–10] and found their application in industrial VOCs oxidizers, produced by Thermatrix [10], ReEco-Stroem [11] and other companies. Physical aspects of the FC in inert porous media are discussed in [4,7,12,13] and other papers.

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Nomenclature

a, a_0	Arrhenius preexponential factor (m^3/(mol s))
C_r	efficiency of recuperation (dimensionless)
C_l	dimensionless losses from sidewall of reactor
c_p	heat capacity of gas (J/(kg K))
c_s	heat capacity of porous carcass (J/(kg K))
$\mathbf{D}$	gas diffusivity tensor (m^2/s)
$\mathbf{D}_d$	dispersion diffusivity tensor (m^2/s)
D_p, D_t	longitudinal and transverse component of dispersion diffusivity tensor
D_g	gas diffusivity coefficient, approximated by nitrogen properties (m^2/s)
d_0	diameter of porous carcass particle (m)
d_1	internal tube diameter (m)
d_2	reactor diameter (m)
G	gas mass flow rate (kg/s)
h_i	mass enthalpy of ith chemical component
Δh	gas mixture heat of combustion (J/kg)
$\mathbf{I}$	unit matrix
k	reaction rate (m^3/(mol s))
k_0, k_1	filtration permeabilities
M	average molecular weight of gas (kg/mol)
m	porosity
p	pressure (Pa)
p_0	outlet pressure (Pa)
Q_r	heat flux via internal tube wall (W)
Q_l	heat losses from side wall of reactor (W)
R	absolute gas constant
r	radius (m)
S	internal tube cross section (m^2)
T	temperature (K)
T_{ad}	adiabatic temperature of combustion, $\Delta T_{ad} = T_{ad} - T_0$ (K)
T_0	initial temperature of the system (K)
U_G	superficial gas velocity (m/s)
$\mathbf{u}$	gas velocity vector (m/s)
X_i	molar fraction of ith component
Y_i	mass fraction of ith component
z_1, z_2	internal tube or reactor length (m)
z_f	combustion front position (m)

Greek symbols

α	heat exchange coefficient (W/(m^2 K))
α_{vol}	volumetric heat exchange coefficient (W/(m^3 K))
ε	emissivity of the porous carcass
ρ	density (kg/m^3)
$\dot{\rho}_i$	mass generation rate of ith component due chemical reactions (kg/s)
Λ	heat conductivity tensor (W/(m K))
λ	conductivity or effective conductivity of porous carcass (W/(m K))
μ	gas viscosity coefficient, approximated by nitrogen properties (Pa s)
σ	Stefan–Boltzmann constant (5.67×10^{-8} W/(m^2 K^4))
$\boldsymbol{\tau}$	unit vector with components τ_z, τ_r
Φ	fuel/air equivalence ratio
Ω	surface of internal tube or reactor sidewall

Subscripts

1	relates to internal tube
2	relates to reactor sidewall
g	gas
i	ith component of gas
s	solid

Though such type of reactors are under investigation and have a practical utilization, there is lack of obtainable publications concerned with detailed parametric study of these devices. The combined regenerator–recuperator scheme of VOC oxidizer was investigated in [14] numerically. Important parameters – maximal temperature of reactor, NO_x emission, effective ranges of gas flow rate and VOC concentration are compared for different types of reactor. It was shown that recuperative–regenerative scheme let one expand the range of operational flow rate and VOC concentration compared to stationary recuperative reactor.

Parametric study of filtration combustion reactor with electro heating elements was presented in [15]. The influence of gas flow rate, electrical heating elements position and power, and thermal isolation on maximal temperature in the system, unburned VOC concentration was investigated.

In this article numerical study of the steady-state recuperative (coaxial tubes type) reactor is performed. The influence of incoming gas flow rate, heat losses via side wall and other parameters on temperature and VOC burning out is under investigation. Reactor recuperation efficiency and combustion front position were under consideration too. The chemical kinetics of the VOC oxidation is modeled by one-step Brutto model for methane combustion.

2. Problem statement

The system under investigation consists of two coaxial tubes, filled with ceramic particles – packed bed (Fig. 1). The reactor walls width is assumed to be zero in the model. The heat losses via side walls may be varied according to Newtonian law (7). At initial time instant porous body (Fig. 1, (4)) was preheated in order to ignite the gas mixture. VOC containing gas (Fig. 1, (1)) enters through central tube, heats up due to the heat exchange with porous body (Fig. 1, (4)) turns-around and goes out through the gap between internal tube and reactor body (Fig. 1, (2)). At certain temperature the VOC oxidation starts and xcombustion products heat up porous media and via it the incoming fresh gas mixture.