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Numerical simulation of heat transfer during production of rutile titanium dioxide in a rotary kiln

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ABSTRACT

This paper presents a computational heat transfer model of a rotary kiln used for the production of rutile titanium dioxide by the calcination of paste-like hydrous titanium dioxide. The work details the modelling of several chemical reactions occurring in the solid bed region along with turbulent convection of gas, radiation heat exchange among hot gas, refractory wall and the solid surface, and conduction in the refractory wall. Finite-difference techniques are used and the steady state thermal conditions are assumed. The kiln is divided into axial segments of equal length. The solution is of marching type and proceeds from the solid inlet to the solid outlet. The direction of gas flow is opposite to that of the solids. Mass balance of each species in the solid charge, and mass and energy balances of the solid and gas in an axial segment are used to obtain solids and gas temperatures, and species concentration at the exit of that segment. The kiln length predicted by the present model is 45.75 m as compared to 45 m of an actual kiln reported by Ginsberg and Modigell (2011). The steady-state axial gas and solid temperature profiles have been also satisfactorily validated with the numerical results of the aforementioned paper. The output data consist of refractory wall temperature distribution, the axial solids and gas temperature profiles, axial solids composition profile, the length required for drying of the solid charge and the total kiln length required to achieve 98% conversion of anatase TiO_2 to rutile TiO_2. A detailed parametric study with respect to the controlling parameters such as percent water content (with respect to dry solids), solids flow rate, gas flow rate, kiln inclination angle and kiln rotational speed lent a good physical insight into the rutile-TiO_2 production process in a rotary kiln.

1. Introduction

This paper presents a computer model of heat transfer during production of titanium dioxide white pigment in rutile form in a rotary kiln.

1.1. Production of rutile titanium dioxide (TiO_2) in a rotary kiln

Titanium dioxide is a white solid inorganic substance which is used as a pigment or whitener in paints, paper, plastics, textiles, and other products. It occurs in several polymorphs, among them, anatase and rutile are manufactured in the chemical industry as white pigments. The pigment properties of rutile titanium dioxide are better than that of anatase titanium dioxide and are of more economical importance. Titanium dioxide white pigments are produced from a variety of ores by two different processes, namely, the sulphate process using concentrated sulphuric acid and the chloride process using chlorine gas. The last process step of the sulphate method, named calcination is performed in rotary kiln and has been considered in the present work.

1.2. Description of rotary kiln

A rotary kiln consists of a refractory lined cylindrical shell mounted at a slight inclination from the horizontal plane (Fig. 1). The kiln is rotated at a very low speed about its longitudinal axis and the raw charge comprising hydrous titanium dioxide in a moist cake form is fed into the upper end of the cylinder and a hot combustion gas mixture at 1 bar flows from the other end. The gas is a mixture of products on burning of natural gas in a separate combustion chamber.

In the present study, the kiln is considered to comprise three sections. In the first section, the wet solids are heated to the saturation temperature of water. In the second section, the liquid evaporates at constant temperature until the charge is completely devoid of moisture. In the third section, the solids are heated till the required degree of conversion of anatase to rutile titanium

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Nomenclature

$A_{e,k}$	frequency factor for kth reaction (s^{-1})
A_{cg}	cross-section area of gas flow in an axial segment (m^2)
A_g	total surface area exposed to gas in an axial segment (m^2)
a_g	gravitational acceleration (9.81 m/s^2)
A_i	elemental area for ith element at inner wall in an axial segment (m^2)
$A_{j,inner}$	contact area between wall and solids per unit element (m^2)
C_p	specific heat at constant pressure (J/kg K)
D	diameter of the kiln (m)
D_h	hydraulic diameter of gas flow (m)
$d\dot{m}_{k,z}$	depletion rate of the reactant of kth reaction in an axial segment (kg/s)
$d\dot{m}_{v,z}$	evaporation rate of moisture content in wet solid in concerned axial segment (kg/s)
$E_{a,k}$	activation energy for kth reaction (J/mol)
E_b	blackbody emission per unit area (W/m^2)
f	percentage of moisture content on dry basis in wet solids
F_{gj}	shape factor between gas and surface element j
F_{ij}	shape factor between surface elements i and j (including $j = i$)
Gr	Grashof number
h_{cgw}	average convective heat transfer coefficient from gas to refractory wall in an axial segment (W/m^2 K)
h_{c_j}	local convective heat transfer coefficient from gas to jth element of solids (W/m^2 K)
h_{fg}	latent heat of vaporization of water (J/kg)
h_o	convective heat transfer coefficient from outer wall to surroundings (W/m^2 K)
h_{ws}	contact heat transfer coefficient between wall and solids (W/m^2 K)
Δh_i	heat of reaction for ith reaction (J/kg)
k	thermal Conductivity (W/m K)
L	length of the kiln (m)
L1	length of the first section of the kiln (m)
L2	length of the second section of the kiln (m)
L3	length of the third section of the kiln (m)
$\dot{m}_{g,z}$	gas mass flow rate at axial position z (kg/s)
$\dot{m}_{k,z}$	mass flow rate of the kth component of solid charge at axial position z (kg/s)
$\dot{m}_{s,z}$	solids mass flow rate at axial position z (kg/s)
Mw_k	molecular weight of kth component of solids (g/mol)
n_k	Order of kth reaction
N	total number of surface elements in an axial segment
N_k	rotational speed of the kiln (rev/min)
N_r	number of surface elements exposed to gas in an axial segment
N_s	number of surface elements covered by solid in an axial segment
Nu_{D_h}	nusselt number based on hydraulic diameter D_h
P_g	wetted perimeter of gas flow in an axial segment (m)
Pr	Prandtl number
$q_{1,z}$	net heat transfer from gas and exposed wall to solids (W)
$q_{2,z}$	net heat transfer from covered wall to solids (W)
$q_{cr,z}$	net heat energy absorbed or released by chemical reactions at axial position z (W)
$q_{gp,z}$	thermal energy associated with the released gaseous products of chemical reactions (W)
q_j	net heat transfer for jth surface element in an axial segment (wall or solids), (W)
$q_{r,z}$	net heat transfer from gas to solids and wall (W)
R	radius of the kiln, Fig. 2
Re_ω	Reynolds number based on relative velocity between wall and air outside the kiln
Re_{D_h}	Reynolds number based on hydraulic diameter D_h
R_u	universal gas constant (8.314 J/mol K)
$T_{g,z}$	gas temperature at axial position z (K)
$T_{j,inner}$	inner wall temperature at jth surface element (K)
$T_{s,z}$	solids temperature at axial position z (K)
Δt	residence time (s)
$T_{o,av}$	average temperature at outer wall (K)
U	circumferential speed of the kiln (m/s)
v_g	mean velocity of gas (m/s)
V_z	axial velocity of solids (m/s)
x	radial coordinate (m), Fig. 2
X_k	mass fraction of the solid component k
y	circumferential coordinate (m), Fig. 2
z	axial coordinate (m)

Greek letters

α	fill angle (deg), Fig. 2
α_{rf}	thermal diffusivity, Eq. (4)
β	volumetric thermal expansion coefficient (K^{-1})
Γ	fill angle (radian)
ε	emissivity
$\zeta_{k,z}$	degree of conversion of kth reaction at axial position z
σ	Stefan–Boltzmann constant (5.67×10^{-8} $W/m^2 K^4$)
θ	as defined in Fig. 2 (deg)
μ	dynamic viscosity (kg/m-s)
ν	kinematic viscosity (m^2/s)
ξ	Darcy friction factor, used in Gnielinski [35] correlation
ρ	density (kg/m^3)
τ_g	transmissivity of the gas
$\Delta\tau$	time step (s)
ϕ	kiln inclination angle (deg)

Subscripts

a	air
cr	chemical reaction
g	gas
gs	gas to solids
i	element number of the wall or the solid
j	element number of the wall or the solid
k	number of reaction, also number of component in solid charge
l	liquid
O_2	oxygen
s	solids
sh	shell or outer wall
SO_2	sulphur dioxide
rf	refractory wall
v	vapour
w	water
ws	wall to solids
z	at an axial distance z from the solids inlet
$z + \Delta z$	at a distance $z + \Delta z$ from the solids inlet

Abbreviations

CFD	Computational Fluid Dynamics