EFFECT OF NOZZLE ASSEMBLY, INSULATION AND OPERATING CONDITION ON PARTIAL COMBUSTION UNIT PERFORMANCE: COMPUTATIONAL FLUID DYNAMICS AND EXPERIMENTAL STUDY

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SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Doctor of Philosophy in Chemical Engineering.

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STUDENT’S DECLARATION

I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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LIST OF SYMBOLS

A	Constant
a	Oxygen reaction order
a_r	Absorption coefficient (1/m)
a_s	Speed of sound (m/s)
a_λ	Spectral absorption coefficient (1/m)
B	Constant
C	Linear-anisotropic phase function coefficient
$C_{1\varepsilon}$	Constant of production rate
$C_{2\varepsilon}$	Constant of destruction rate
$C_{3\varepsilon}$	Coefficient of production rate
C_μ	Coefficient of turbulent viscosity
c	Progress variable
c_p	Specific heat capacity (J/kg·K)
D	Diameter (m)
$D_{i,m}$	Diffusion coefficient (m^2/s)
D_t	Turbulent diffusion coefficient (m^2/s)
E	Energy (J/kg)
f	Correction factor
$\overline{f}$	Mean mixture fraction
G	Incident radiation flux (W/m)
G_b	Production term due to turbulence buoyancy
G_k	Production term of turbulence kinetic energy
g_i	Gravitational vector
h	Convective heat transfer coefficient ($W/m^2 \cdot K$)
$I_{b\lambda}$	Black body intensity ($J/m^2 \cdot s$)
I_λ	Spectral radiation intensity ($J/m^2 \cdot s$)
k	Turbulent kinetic energy (m^2/s^2)
k	Thermal conductivity (W/m·K)
k_{f1}, k_{f2}, k_{f3}	Rate constant for forward reactions (m^3/mol·s)
k_{r1}, k_{r2}, k_{r3}	Rate constant for reversible reactions (m^3/mol·s)
k'_{pr}	Rate constant for prompt NO (m^3/mol·s)
L	Length scale in SAS model
L_{vk}	Von Karman length scale
M_t	Mach number

$M_{w,i}$	Molecular weight of combustion species (g/mol)
$M_{w,j}$	Molecular weight of product species (g/mol)
$M_{w,R}$	Molecular weight of reactant species (g/mol)
N	Total species
Nu	Nusselt number
n	Number of carbon atoms in fuel molecule
n	Refractive index
P	Pressure (Pa)
P_k	Production rate term in SAS model
Pr_t	Turbulent Prandtl number
Q	Q-criterion
$\dot{Q}$	Rate of heat transfer (W/m^2)
$\dot{Q}_{Cond}$	Rate of conduction (W/m^2)
$\dot{Q}_{Conv}$	Rate of convection (W/m^2)
$\dot{Q}_{Rad}$	Rate of radiation (W/m^2)
q	Heat flux (W/m^2)
q_r	Radiation heat flux (W/m^2)
R	Gas constant (J/mol·K)
R_i	Net production of chemical reaction rate (kg·mol/m^3·s)
Re	Reynolds number
r	Reaction
$\vec{r}$	Radiation position (m)
S	Mean strain rate
S_E	Source term for energy conservation equation
S_i	Additional term
S_M	Source term due to body force
S_{user}	Source term
Sc_t	Turbulent Schmidt number
s	Path length (m)
$\vec{s}\,'$	Radiation direction
T	Temperature (K)
T_g	Gas temperature (K)
T_r	Radiation temperature (K)
T_s	Wall surface temperature (K)
t	Time (s)

U_t	Turbulent flame speed (m/s)
U'	Invariant of strain rate tensor
u_∞	Free-stream flow velocity (m/s)
u_x	Axial or streamwise velocity (m/s)
u_y	Radial velocity (m/s)
u_z	Tangential or crossflow velocity (m/s)
$u*$	Normalized mean velocity
$\overline{u_i' u_j' u_k'}$	Reynolds stresses
v	Velocity in y direction (m/s)
$v''_{j,r}$	Product species stoichiometric coefficient
$v'_{R,r}$	Reactant species stoichiometric coefficient
X	Length of PCU in x direction (m)
x	Thickness (m)
Y	Length of PCU in y direction (m)
Y_i	Mass fraction of species
$Y_{i,eq}$	Equilibrium mass fraction
Y_M	Dilatation dissipation term
Y_P	Mass fraction of product species
Y_R	Mass fraction of reactant species
y^+	y-plus function
w	Velocity in z direction (m/s)
Z	Length of PCU in z direction (m)
ρ	Density of fluid (kg/m^3)
ρ_u	Density of unburnt mixture (kg/m^3)
τ	Viscous stress (N/m^2)
μ	Viscosity of fluid (kg/m·s)
μ_s	Viscosity of fluid at wall surface (kg/m·s)
μ_t	Turbulent viscosity (kg/m·s)
σ	Stefan-Boltzmann constant (W/m^2·K^4)
σ_k	Turbulent Prandtl-Schmidt number for turbulent kinetic energy
σ_s	Scattering coefficient (1/m)
σ_ε	Turbulent Prandtl number for turbulent dissipation rate
σ_ϕ	Turbulent Prandtl number for SAS model
ε	Turbulent dissipation rate (m^2/s^3)
ε_r	Emissivity
β	Coefficient for G_b

β	Thermal expansion coefficient
γ	Ratio of specific heat
δ	Viscous stress tensor (N/m^2)
θ	Coefficient
Ω_k	Rotation vector
Φ	Coefficient in SAS model
ϕ	Phase function
ϕ	Equivalence ratio
ϕ	Scalar variable
$\overline{\phi}$	Mean component
ϕ'	Fluctuating component
λ	Wavelength (m)
λ_2	Lambda-2
Ω	Vorticity magnitude
$d\Omega'$	Solid angle
$\zeta_1, \zeta_2, \zeta_3$	Constant

LIST OF ABBREVIATIONS

CCD	Charge-coupled device
CFD	Computational fluid dynamics
CPU	Computer processor unit
DES	Detached eddy simulation
DGV	Doppler global velocimetry
DNS	Direct numerical simulation
DO	Discrete ordinates
DTRM	Discrete transfer radiation model
EBU	Eddy break-up
EDC	Eddy dissipation concept
EDM	Eddy dissipation model
ELPI	Electrical low pressure impactor
FFT	Fast Fourier transformation
FGM	Flamelet-generated manifold
FR	Finite rate
FTIR	Fourier transform infrared
GRI	Gas Research Institute
HWA	Hot wire anemometry
JP8	Jet propellant 8
KSKL	K-square-root-K-L model
LDA	Laser Doppler anemometry
LDV	Laser Doppler velocimetry
LES	Large eddy simulation
PCU	Partial combustion unit
PDF	Probability density function
PIV	Particle image velocimetry
PLLIF	Planar, liquid laser-induced fluorescence
PRESTO	Pressure staggering option
P-1	Spherical harmonics
QUICK	Quadratic upwind interpolation scheme for convective kinematic
RANS	Reynolds-averaged Navier-Stokes
RKE	Realizable k-ε
RNG	Renormalized k-ε
RSM	Reynolds stress model

SAS	Scale adaptive simulation
SKE	Standard k-ε
SST	Shear stress transport
S2S	Surface-to-surface
URANS	Unsteady Reynolds-averaged Navier-Stokes
WSGGM	Weighted sum of gray gas model

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ABSTRAK

Pembakaran separa syngas sering digunakan untuk menghasilkan besi yang berkualiti tinggi di kilang pemprosesan keluli. *Partial combustion unit* (PCU) mengalami masalah kekurangan suhu tinggi yang disebabkan oleh reka bentuk yang tidak sesuai and kehilangan haba. Ini menyebabkan bahan api yang banyak dan kos operasi yang tinggi diperlukan untuk mengekalkan kualiti besi. Oleh itu, pengubahan reka bentuk PCU adalah penting untuk mencapai prestasi pembakaran yang lebih baik dan untuk mengurangkan penggunaan bahan api. Penyelidikan ini bertujuan untuk menangani isu-isu tersebut dengan mencadangkan beberapa reka bentuk muncung baru dan memasang penebat haba pada PCU yang sedia ada. Tiga reka bentuk muncung baru telah dicadangkan untuk memastikan pencampuran bahan api yang lebih baik, manakala empat penebat haba yang berbeza (iaitu, batu bata, besi tuang, gentian seramik dan fabrik grafit) telah diuji untuk mengurangkan kehilangan haba. Ujian eksperimen tidak boleh digunakan jika dinding PCU legap, oleh itu teknik *computational fluid dynamics* (CFD) digunakan untuk mengkaji aliran bendalir reaktif dan pemindahan haba dalam PCU. Simulasi CFD dalam PCU adalah sukar sebab ia melibatkan suhu tinggi serta gandingan antara pergolakan, tindakbalas kimia dan pemindahan haba. Oleh itu, simulasi CFD perlu disahkan sebelum ia boleh digunakan secara rutin. Pengesahan tersebut dilakukan pada PCU yang berskala kecil dengan menggunakan pengukuran LDV, serta dengan membandingkan kiraan CFD dengan pengukuran yang telah diterbit. Tiga model pergolakan, iaitu *standard k-ε* (SKE), *Reynolds stress model* (RSM) dan *scale-adaptive simulation* (SAS) telah digunakan. Tindak balas pembakaran telah dimodelkan dengan menggunakan *eddy dissipation model* (EDM) dan *flamelet model* bersama dengan tindakbalas kimia terperinci, manakala pemindahan haba dihitung dengan mempertimbangkan perolakan, konduksi dan radiasi. Model *discrete ordinates* (DO) dan *spherical harmonics* (P-1) telah digunakan untuk menghitung pemindahan haba secara sinaran. Saluran masuk daripada PCU dan muncung diambilkira sebagai halaju masuk bersama dengan campuran species, manakala dinding dianggap sebagai sempadan yang tidak tergelincir. Keputusan kajian menunjukkan bahawa *non-premixed flame model* bersama dengan tindakbalas kimia terperinci memberi ramalan tepat dengan sisihan 6.58%. Ramalan tanpa mempertimbangkan radiasi didapati menyebabkan sisihan > 9% berbanding dengan hanya < 7% apabila sinaran dimodelkan. Model DO memberikan ramalan yang terbaik untuk pemindahan haba sinaran dengan sisihan 5.65%. Selain itu, semua model pergolakan memberi ramalan yang baik pada suhu saluran keluar dengan sisihan yang kurang daripada 6% berbanding pengukuran eksperimen. Tetapi, SAS memberikan ramalan yang terbaik dengan sisihan 5.25%. Semua reka bentuk muncung baru menghasilkan suhu 11% lebih tinggi daripada reka bentuk asal, di mana muncung bersama dengan sayap bermukaan rata memberikan prestasi pembakaran yang terbaik dengan peningkatan suhu puncak lebih 45% daripada PCU asal. Penambahan 40% kadar aliran oksigen didapati meningkatkan suhu puncak kira-kira 12%. Operasi muncung berkembar didapati lebih berkesan daripada operasi muncung tunggal pada kadar aliran oksigen yang sama. Di samping itu, pemasangan penebat haba meningkatkan lebih 17% daripada suhu puncak di saluran keluar. Penebatan terbaik telah dicapai dengan menggunakan gentian seramik dengan suhu puncak 20.4% lebih tinggi daripada PCU asal. Hasil daripada penyelidikan ini boleh berguna untuk reka bentuk naik taraf PCU, dimana CFD model boleh diguna untuk mensimulasikan prestasi PCU dan data LDV diguna untuk pengesahan.

ABSTRACT

Partial combustion of syngas is often used to produce high-quality metallic iron in steel processing plant. Partial combustion unit (PCU) suffers from insufficient high temperature due to improper design configuration and heat loss. Consequently, higher rate of fuel injection and operating cost is required to maintain the quality of iron. Hence, a proper retrofit of design on the PCU is vital to offer better combustion performance and to reduce fuel consumption. This work aims to address the issues by proposing several new nozzle assembly designs and by installing thermal insulator to the existing PCU. Three new nozzle assembly designs were proposed to offer better turbulent mixing, whereas four different thermal insulators (i.e., brick, iron cast, ceramic fibre and graphite felt) were tested to minimize the heat loss. Experimental measurement is not applicable for opaque wall of PCU and hence computational fluid dynamics (CFD) technique is used to study the reactive fluid flow and heat transfer in the PCU. CFD simulation of the PCU at extreme temperatures is challenging owing to the coupling between the turbulence, chemistry and heat transfer. Hence, a CFD simulation must be validated before it can be routinely used. The validation was performed using the LDV measurement of a scale-down PCU rig, as well as by comparing with the published measurements. Three turbulence models, namely standard k-ε (SKE), Reynolds stress model (RSM) and scale-adaptive simulation (SAS) were employed. Combustion reaction was modelled using the eddy dissipation model (EDM) and detailed chemistry flamelet models, whereas the heat transfer was calculated by considering a convection, conduction and radiation. Discrete ordinates (DO) and spherical harmonics (P-1) were used for radiative heat transfer. The inlet of PCU and nozzle is treated as inlet velocity with species mixture while the wall is assumed as non-slip boundary. The finding showed that the non-premixed flame model with detailed chemistry provided a better prediction with 6.58% of deviation from measured temperature. It was found that the prediction without considering radiation yielded over 9% error compared to < 7% error when radiation is modelled. The DO model gave the best prediction of radiative heat transfer with 5.65% of deviation. Besides that, all turbulence models provided a good prediction of outlet temperature with a deviation of less than 6% from measured data. However, SAS gave the best prediction with 5.25% of error. All new nozzle assembly designs achieved over 11% higher temperature where the nozzle with flat surface wing gave the best performance with over 45% increase in temperature than the original wingless PCU. It was found that 40% increase in oxygen flowrate increased the peak temperature by about 12%. Dual-lance was found more effective than the single-lance operating at a similar oxygen flowrate. In addition, installation of insulation enhanced over 17% of peak outlet temperature. The best insulation was achieved using ceramic fibre with 20.4% higher peak temperature than the original non-insulated PCU. The finding from this work may useful for design retrofitting of a PCU, whereby the CFD model can be employed to simulate the PCU performance and the LDV data can be used for validation.

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