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PROCESS SIMULATION AND SENSITIVITY ANALYSIS OF INDIRECT COAL GASIFICATION USING ASPEN PLUS® MODEL

Fahim Uddin[1, 2], Syed A. Taqvi[1, 2] and Inayatullah Memon[2]
[1]Department of Chemical Engineering, Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskander, Perak, Malaysia
[2]Department of Chemical Engineering, NED University of Engineering & Technology, Karachi, Pakistan
E-Mail: fahim_nedian@yahoo.com

ABSTRACT

A steady state Aspen Plus® simulation is used to propose and analyse a novel indirect gasification model using steam as the gasifying medium. A sensitivity study is carried out by varying the steam-to-coal ratio. Part of the Syngas produced is combusted in the furnace to provide flue gases at high temperature which is then passed through the bayonets to provide reaction heat. RK-Soave method is used for the evaluation of physical properties of mixed conventional components and CISOLID components in the simulation. The feedstock used in the simulation is indigenous Thar coal from Pakistan, where large coal reserves are present. It was found that a lower steam-to-coal ratio increases the heat content of the syngas produced. Also, the carbon conversion undergoes a maximum at the ratio 2.0. As we increase the steam-to-coal ratio, the yields are better but inevitably reduce the quality of syngas produced. Carbon conversions and H_2/CO ratios as high as 95.76% and 3.09 respectively were observed with higher steam to carbon ratios. However, lower ratios provide high yields (69.00%) and cold gas efficiencies (54.41%). Based on these results, it can be said that this parameter significantly influences the syngas quality and processing costs and the diversity of trends suggest a more detailed analysis for optimisation of the process.

Keywords: aspen plus, coal, energy, gasification, syngas.

INTRODUCTION

Last century was transfigured by the discovery of petroleum and natural gas and so far they have been fuelling our world. However, their depletion is at hand and thus high prices are pinning the industries to move on to other fuels. Oil is currently fuelling 33% of the market, a remarkable decrease from 48% in 1973. Especially for power generation, the oil's contribution has fallen to 4% (BP Energy Outlook 2030, 2012). It is high time to work on other energy sources and find the alternates of petroleum and natural gas. Coal is one of the world's most important sources of energy regarding its abundance and variety of possibilities for processing (The Coal Resource: A Comprehensive Overview of Coal, 2005). The biggest market for coal is Asia, which currently accounts more than half of global coal consumption (BP Energy Outlook 2035, 2015). Coal plays a vital role in power generation and this role is set to continue. Its share of electricity production worldwide has increased from 40% to 44% in last two years (BP Energy Outlook 2030, 2012), (BP Energy Outlook 2035, 2015).

Gasification is a clean coal technology with better environmental performance than coal combustion as its reducing environment aids to isolate, capture and utilise the reduced forms of sulphur and nitrogen (Phillips, 2006). If the process does not occur with an oxidising agent, it is called indirect gasification and needs an external energy source (Rocca, 2003). Steam is frequently used indirect gasification agent because it is easily produced and increases the hydrogen content of the combustible gas (Sudiro, 2010). This also results in a better calorific value of the syngas produced due to the presence of high CH_4 content (Sudiro, 2010).

Modelling of fixed bed gasifiers has not been exhausted yet, to say the least. Hobbs (Hobbs et al., 1992) modelled a counter-current fixed bed gasifier, the results of which were compared with the commercial gasifiers. Radulovic (Radulovic et al., 1995) further amended its devolatilization model. Grieco (Grieco and Baldi, 2011) removed the assumptions of temperature uniformity among particles and absence of radiation during gasification.

To provide energy for indirect gasification, a bayonet heat exchanger is used within the gasifier (Akhlas et al., 2015a). This layout allows the usage of high-temperature heating streams (combustion exhaust gases up to 1400°C) and suitability in the environments with high-temperature differences (O'Doherty et al., 2001). The heat transfer model used is based on the one presented by Bussman (Bussman, 2005) for cooling bayonets of testing burners in industries.

In this paper, a sensitivity analysis of indirect coal gasification process by means of steam as the gasifying medium is conducted. Here coal is fed to the reactor along with the steam where gasification takes place. Reaction heat is supplied by the bayonets installed in the reactor. A fraction of Syngas is combusted to provide hot combustion exhaust gases which are then passed through the bayonets for heat integration. The models for the gasifier and heat integration are established using Aspen Plus® software and Microsoft Excel®.

PROCESS MODEL

Components

The species used in this simulation were O_2, CO, H_2, CO_2, H_2O, CH_4, N_2, H_2S, Tar (as C_6H_6*), C (solid) and S (solid). Non-conventional components in the simulation were defined by their Proximate, Ultimate and Sulphur

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Analyses to represent coal, dry coal, char and ash. Thar coal has been defined in Table-1 (Jaffri and Zhang, 2009).

Table-1. Analysis of Thar coal.

Proximate analysis		Ultimate analysis		Sulphur analysis	
Element	**wt.%**	**Element**	**wt.%**	**Element**	**wt.%**
Moisture (wet basis)	8.5	C	54.57	Pyritic	1.46
		H	3.21		
FC (dry basis)	25.83	N	1.07	Sulphate	1.47
		Cl	0		
VM (dry basis)	53	S	4.39	Organic	1.46
		O	15.59		
Ash (dry basis)	21.17	Ash	21.17		

Process description

The schematic diagram of the gasifier is shown in Figure-1. In this process, coal and steam are mixed and fed to the reactor where gasification occurs. Reaction heat is provided by the bayonets which are nearly vertically installed in the reactor. The gases thus produced are CO, CO_2, H_2 and CH_4. Some unreacted steam also accompanies them in the product stream. The ash produced along with the unreacted char in the reaction is drawn off through the bottom. The Syngas produced in the reaction is divided into two parts. A fraction of the Syngas is combusted to provide hot combustion exhaust gases which then pass through the bayonets for heat integration.

In the upper section of the gasifier, adiabatic processes such as drying, pyrolysis and some gasification of the char take place. The energy necessary for these processes is delivered by the product stream passing through this section at a higher temperature until the thermal equilibrium is established.

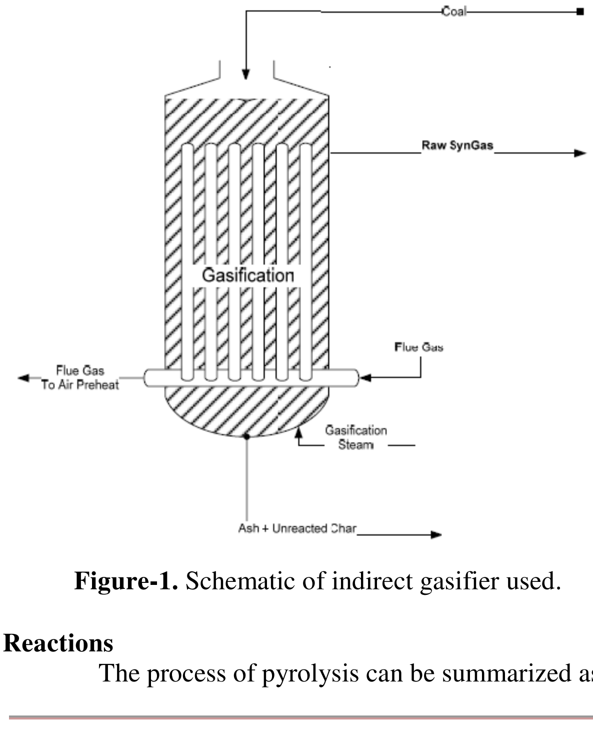

Figure-1. Schematic of indirect gasifier used.

Reactions

The process of pyrolysis can be summarized as:

$$Coal \rightarrow CO + CO_2 + CH_4 + C_6H_6 + H_2 + H_2O + H_2S + N_2 + Char \quad (1)$$

Following reactions are considered in the process of char gasification (Wen *et al.*, 1982) (Rinard and Benjamin, 1985).

$$C + \frac{z+2}{2z+2} O_2 \rightarrow \frac{z}{z+1} CO + \frac{1}{z+1} CO_2 \quad (2)$$

$$C + CO_2 \rightarrow 2CO \quad (3)$$

$$C + H_2O \rightarrow CO + H_2 \quad (4)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (5)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (6)$$

$$CO + 2H_2 \rightarrow CH_4 \quad (7)$$

Where z in Equation 2 is defined as: (Wen and Chaung, 1979),

$$z = \frac{[CO]}{[CO_2]} = 2500e^{-6249/T} \quad (8)$$

The reactions defined for char gasification are mainly of two categories; gas-solid and gas-gas. In the solid-gas reaction (1), the rate of reaction is usually fast relative to diffusion rate of oxygen into the coal volume; therefore this reaction is characterised as the surface reaction. Reactions (2)-(4) have rather slow rates of reactions at the gasifier temperature below 1000°C, thus they are volumetric in nature.

Assumptions

Following assumptions were taken into account while developing this model:

a) The process is in steady-state with negligible pressure losses;
b) Solid and gaseous phases are in thermal equilibrium;
c) The pyrolysis gas leaves the reactor without passing in the area of char gasification.

Heat Integration

Raw Syngas is available from the gasifier at sufficiently higher temperature than the temperature required for further processing and purification. To utilise this excess heat, it is introduced in a cross flow heat exchanger to produce saturated steam from water. The stream is further sent for superheating. The cooled syngas is now fragmented into two parts, one of which is drawn as product for supplementary treatment. The other part is mixed with the preheated air to be combusted.

The mixture of syngas and hot air is fed to the furnace. As a result, hot combustion exhaust gases are produced. The saturated steam produced in the Complementary Steam Generation and Syngas cooling sections utilises the heat from the hot furnace gases and produce high-pressure superheated steam. This steam is introduced in the gasifier for the main process.

After leaving the bayonets, the combustion exhaust gas stream preheats the air which is needed for syngas combustion in the furnace. Then it further loses its heat content in order to produce saturated steam as a process utility. This steam is mixed with the steam coming from the Syngas Cooler to be further heated to superheated steam. Cooling of the available ash preheats the water circulating the cooler jacket.

NUMERICAL MODELLING

Bayonet heat exchanger model in the gasifier is based on the one presented by Bussman (Bussman, 2005). It consists of a number of bayonet tubes installed vertically. Each tube consists of two parts. The inner part or the centre tube is made of ceramic in which hot combustion exhaust gases are introduced from the bottom and rise to the top. Then the gases turn around and flow down the metallic annular section and leave the bayonet to join the structure at downstream. The geometry of the bayonet tubes distribution in the gasifier is supported by a representation in Figure-2. Following assumptions are taken into account while developing the calculation model for heat transfer from the bayonet tubes to the reactor.

a) Thermal properties of the gas streams in each cell are calculated at its mean temperature.
b) Heat transfer is primarily radial, thus heat transfer in axial direction can be neglected.
c) The coal flows axially in the tube heat exchanger.
d) Radiation heat transfer occurs from the wall of centre pipe to the inner wall of the annulus and from outer wall of annulus to the reactor volume.

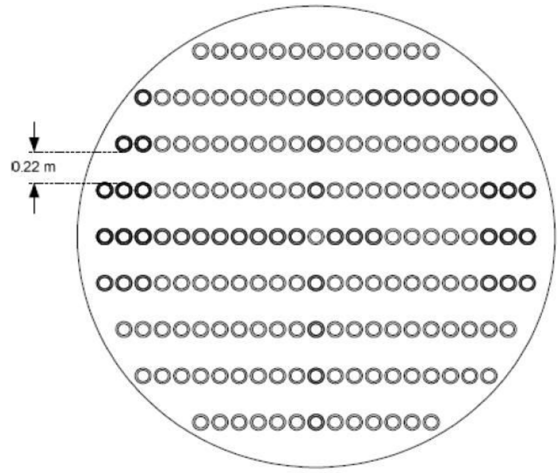

Figure-2. Distribution of bayonets across the reactor cross-section.

The energy balance equations are designed for each cell 'i' of the bayonet tube by considering the three modes of transference of heat i.e., radiation, convection and conduction. The zones of transfer were the centre pipe, annular section and gasifier environment. Total heat transferred to the gasifier and between adjacent cells was also considered (Taqvi *et al*., 2015).

The combustion exhaust gas properties (C_p, μ, k, and ρ) passing through the bayonet heat exchangers and properties of the syngas-steam mixture flowing over the bayonets are retrieved from the properties of streams. The volume flow rate over the bayonet surface and heat transfer q_i for each cell are also brought into agreement with the heat transfer taking place in the gasifier reactors, in the Aspen Plus® scheme.

The model for energy balance developed is designed in Microsoft Excel®. In the topmost portion of the bayonet, an assumption is made that gases leaving the centre pipe and entering the annular section are in thermal equilibrium and heat losses in the top hemispherical section can be ignored. Residual for each cell is calculated to be minimised for each equation.
The system of six equations is then resolved to find the temperature profiles in the gasifier.

RESULTS AND DISCUSSIONS

The feedstock of the gasification process is given in Table II. The Lower Heating Value (LHV) of Thar Coal is found to be 4979 kCal/kg (8956 Btu/lb) by a correlation presented by Mason and Gandhi (Mason and Gandhi, 1983).

$$Q = 44.95A + 198.11C + 620.31H + 80.93S - 5153 \quad (9)$$

The pyrolysis yield for Thar coal is devised on the basis of ultimate analysis and their comparison with the pyrolysis yield for Thar Coal.

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Table-2. Feedstock conditions for the gasification process of Thar coal.

COAL	Pressure	34	bar_g
	Temperature	293	K
	Particle Diameter	2.0	cm
STEAM (Gasifying medium)	Pressure	34	bar_g
	Temperature	1073	K

There is a direct effect of heat transfer on the reaction kinetics by altering the temperature profiles and thus conversion of the reactor. So, the simulation model of gasification kinetics on Aspen Plus® is merged with the energy balances in Microsoft Excel® and the heat integration scheme again in Aspen Plus®. The height of each bayonet is divided into 12 cells, and all of these are modelled for heat balance equations. The gasifier is modelled by a CSTR battery, each corresponding to the particular bayonet heat exchanger cell. Each portion of the reaction is characterised by a single average temperature. As a result of this temperature consistency, CSTR reactors are used to model the different portions of the gasifier.

Heat integration simulation in Aspen Plus® is used to find entering and exiting properties of the combustion exhaust gases across the bayonets.

The volumetric flow rate and physical properties of combustion exhaust gas are temperature-dependant parameters. In recognition of this fact, specified correlations for these parameters are defined. Using the values from the simulation, temperature dependencies of density ρ, specific heat C_p, dynamic viscosity μ and thermal conductivity k of combustion exhaust gases are defined as its linear function.

For any given cell with temperature T (K), the Dynamic Viscosity (Pa.s.) is given as:

$$\mu = C * T^{0.5} \tag{10}$$

The models are run in an iterative sequence to find a temperature and energy distribution which satisfies all of them.

Figures 3 and 4 respectively present the typical trends of temperature profile and heat distribution profile in the bayonets along the length. This representation shows that the combustion exhaust gases entering the bayonet centre pipe cool down, giving away heat to the cooler gases in the annular section which subsequently transfers this heat to the endothermic gasification reaction taking place over the surface of bayonets. Also, an increasing trend is observed in the temperature profile of the gases in annular section.

The temperature of the incoming gasifier gases drastically increase in only one-third of the bayonet height due to the heat provided by the hot combustion exhaust gases and due to some combustion in char because of high oxygen content.

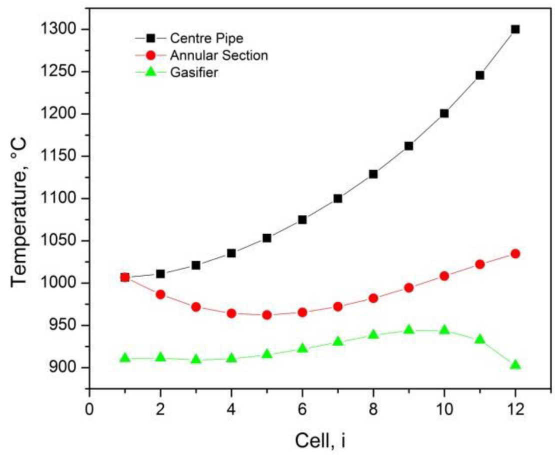

Figure-3. Temperature profiles along the length of the gasifier.

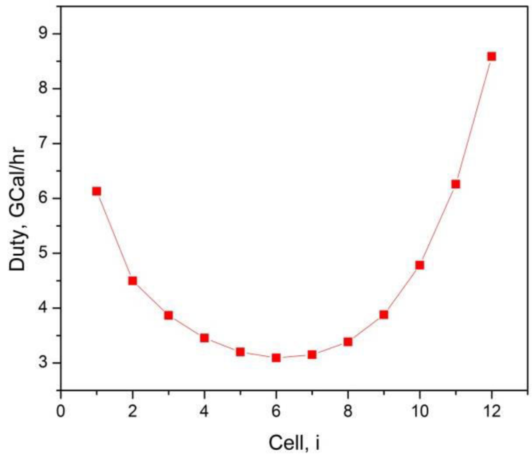

Figure-4. Heat distribution profiles along the length of the gasifier.

Terminologies

The terms which were used to analyse and compare the simulations performed are as follows.

Conversion

The term 'Conversion of coal' refers to the fraction of carbon content in the char converted to that entering the reactor.

$$X_C = \frac{m_{c,in} - m_{c,out}}{m_{c,in}} \tag{11}$$

Product split

Product Split is the part of syngas initially leaving the gasifier which has to be combusted in the furnace.

Excess air

Air flow rate in the furnace for syngas combustion is kept at 60% in excess to the stoichiometric air required. The air flow rate in the Aspen Plus® heat integration scheme is calculated as:

$$n_{air} = \frac{100}{21} \times 1.6 \times \left(0.5n_{CO} + 0.5n_{H_2} + 7.5n_{C_6H_6} + 0.5n_{CH_4}\right) \quad (12)$$

Cold Gas Efficiency

$$ColdGasEfficiency = \frac{TotalHeatingValueOfDrySyngas}{LHVofTotalWetCoal} \quad (13)$$

Syngas Yield

$$SyngasYield = \frac{MassFlowrateOfDrySyngas}{MassFlowrateofCoalFeed} \quad (14)$$

Steam-to-Coal Ratio

$$Steam-to-Coal-Ratio = \frac{MassFlowrateOfSteam}{MassFlowrateOfCoalFeed} \quad (15)$$

Condensate

Condensate may be defined as the water which is condensed and removed from syngas at elevated pressure. A wastewater treatment is essential for such a stream.

Sensitivity analysis

Simulation trials were conducted by varying the steam to coal ratio by changing the coal flow rate whereas the steam flow rate and all other parameters were kept constant.

Figure-5 shows important results obtained from the study. Three parameters i.e. Condensate/Syngas ratio, Carbon conversion and H_2/CO ratio are plotted against the steam-to-coal ratio for analysis. It can be observed that H_2/CO molar ratio has an increasing trend in the selected range of steam-to-coal ratio. Hence it can be deduced that a large steam-to-coal ratio escalates the syngas heat content. Also, an increasing trend in the carbon conversion was observed when a large steam-to-coal ratio was used. Hence it can be concluded that carbon conversion increases with the increase in the steam-to-coal ratio. Nevertheless, other ratios can be advantageous if the unconverted char is also burnt in the furnace to produce hot combustion exhaust gases, which can, in turn, reduce the syngas requirements to provide hot combustion exhaust gas in the bayonets. This alternate scheme has also been studied by Akhlas (Akhlas *et al.*, 2015b). A sensitivity analysis of that scheme will further clarify the influence of steam-to-coal ratio on this gasifier.

It is also shown that the ratio 2.0 has the least Condensate/Syngas ratio. A lesser value of this ratio leads to a relatively lesser condensate production, hence lower wastewater treatment costs.

Figure-6 shows some other significant results. Three parameters i.e. Syngas yield, Cold gas efficiency are plotted against the steam-to-coal ratio for analysis. The yield of syngas and product split ratio were found to have a decreasing trend. Thus it can be concluded that as we increase the steam-to-coal ratio, the yields decline. However, the amount of syngas needed to be burnt in the furnace also reduces, so overall yield can be optimised. The plausibility of this outcome can be inferred by the increase in the H_2 content of the syngas produced. It is interesting to note that use of excess steam does increase the Cold gas efficiency of syngas.

Last but not the least is the LHV of syngas produced as shown in Figure-7. It is evident that this criterion has a decreasing trend.

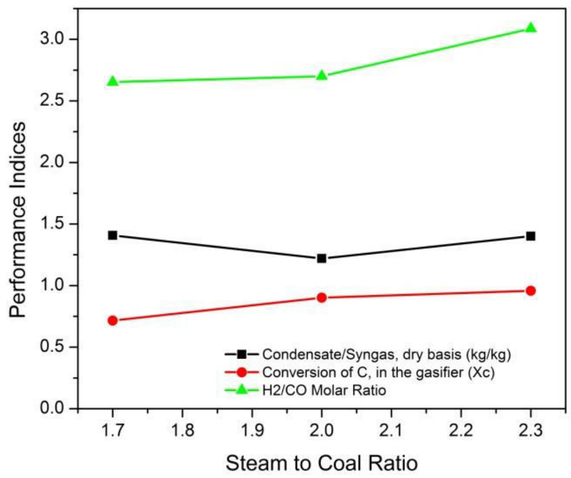

Figure-5. Steam-to-coal ratio analysis: comparison of parameters (a).

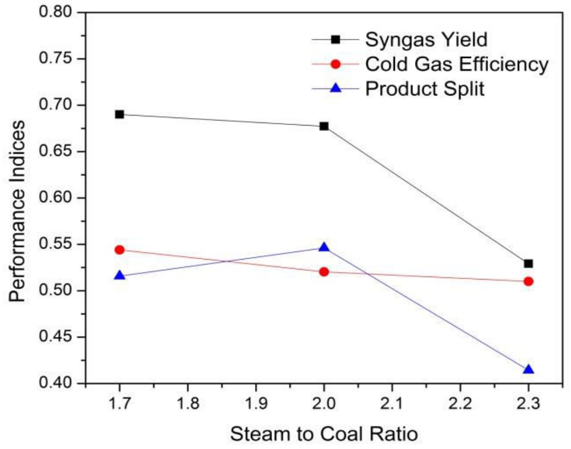

Figure-6. Steam-to-coal ratio analysis: Comparison of Parameters (b).

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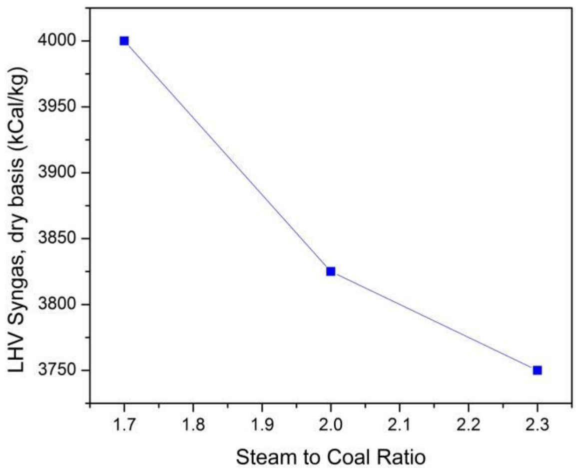

Figure-7. Steam-to-coal ratio analysis: comparison of parameters (c).

CONCLUSIONS

In this work, a novel scheme for indirect gasification of coal using steam was proposed. The heat required for gasification was provided using the vertical bayonets fitted in the reactor. Some of the produced syngas was burned in the furnace and fed into the bayonets. The model for this process was developed using Aspen Plus® simulator, which is extensively used in modelling new process schemes and analysing their potential. Sensitivity analysis was carried out by varying Steam-to-coal ratio of the feed. Seven quality parameters were defined for assessment.

It was found that this parameter does have a significant effect on the important parameters used for comparison. Therefore, it can significantly affect the quality of syngas produced and the processing costs incurred. Different performance criteria indicate different values for their enhancement. Hence there is a need for detailed analysis in this regard by increasing the number of observations and range to study this effect in further detail. This will lead to a better optimisation of this parameter for the process, hence improving the feasibility of the proposed scheme.

Nomenclature

T	= Temperature, K.
C_p	= Specific heat of combustion exhaust gas, J/kg.K.
[CO]	= Mean concentration of CO,
[CO_2]	= Mean concentration of CO_2,
k	= Thermal conductivity of combustion exhaust gases, W/m.K.
μ	= Dynamic Viscosity of combustion exhaust gases, Pa.s.
$\dot{m}$	= Mass flow rate of combustion exhaust gases, kg/sec.
LHV	= Lower Heating Value
ρ_1	= Density of Inlet exhaust Gases FG1300, kg/m^3
q_i	= Heat provided by cell ‘i’ of a tube, W/tube

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