Catalytic Phenol Oxidation with Phase Change in a Periodically Operated Trickle Bed Reactor

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Abstract **- Catalyst wet air oxidation (CWAO) are studied experimentally in this work using a trickle bed reactor operating over $0.5\%Pt/\gamma$-Al_2O_3 catalyst in a steady state and periodic operation mode; ON-OFF liquid flow modulation. The effects of cycle period and split on conversion performance enhancement, were examined at various operating conditions including space time, superficial gas velocity and bed temperature. The results shown that periodic liquid flow modulation can enhances CWAO of phenol with phase change to a maximum value 100% phenol time average conversion at 0.25 cycle split ,9min cycle period , 0.8h space time and 165 ºC bed temperature , while it drops to lower steady state value with longer periods. According to the kinetic results, the reaction behavior was pseudo first order with respect to phenol and kinetically controlled and efficient mineralization of phenol (total oxidation to CO_2) occurs for steady state operation while partial oxidation of phenol to intermediates compounds of low molecular weight carboxylic acids for periodic operation especially at 2 min, 0.25 split and 9 min, 0.25 split.**

Keywords: Trickle-bed reactor; Periodic operation, Phenol oxidation, Catalytic wet air oxidation, Reaction kinetics.

1. Introduction

The most common pollutants are the phenol and phenolic compounds which presents in the wastewaters from oil refineries, coal conversion processes and pharmaceutical industrial processes, therefore, these pollutants need to be treated before its release [1].Aqueous wastes of phenol and phenolic pollutants load in the range of 500-5000 ppm are too toxic and concentrated for a biological treatment, so that, within this niche of concentrations and toxicity, so that catalytic wet air oxidation (CWAO) has been shown to be an suitable destruction technique for the advantages lie in the low operating costs due to the mild requirement of pressure and temperature[2-3].In most CWAO processes fall into the category of catalytic three phase reactions and fixed-bed reactors (TBRs) have been favored over slurry or fluidized reactors, therefore; their multi-phase character forms a great deal of chemical reactor engineering and design challenges as the overall outcome of such processes rely in a complex manner on the interphase and intraparticle diffusion, chemical kinetics, thermodynamics, flow regimes and hydrodynamics [4-5].In trickle-bed reactor operated in trickling regime, liquid evaporation may occurs, which makes possible a compose of dry region in catalyst pellets, then the reaction takes place on dry catalyst surfaces and various possible situations of the catalytic pellet can result from the evaporation of liquid flowing over the external catalyst surface. Within the external trickling liquid film, an enormous portion of the overall mass transfer resistance disappears, due to the much higher reactant diffusion coefficients in the gas phase than in the liquid phase, the internal surface of catalyst obtains extra efficient use [6-7]. The TBRs can be operated under cyclic (periodic/unsteady state) operation, in which one or more operating parameters are periodically varied in time where in periodic operation the system is forced a reacting to operate continuously in a transient mode such as liquid flow modulation [8-9].It is required to enhance the mass transfer characteristics of the limiting reactant in multiphase reactors (TBRs), so that, periodic operation technique seems to be a favorable tool to enhance the performance of TBRs by cyclic liquid operation (ON-OFF cycling) which can be accomplished by pulsing directly the liquid loading, i.e. switching the liquid flow rate between a minimum set zero in OFF period and a maximum value in ON period. [9-12].Since 1989, there are many studies on the liquid flow modulation operation to detect the transient behavior

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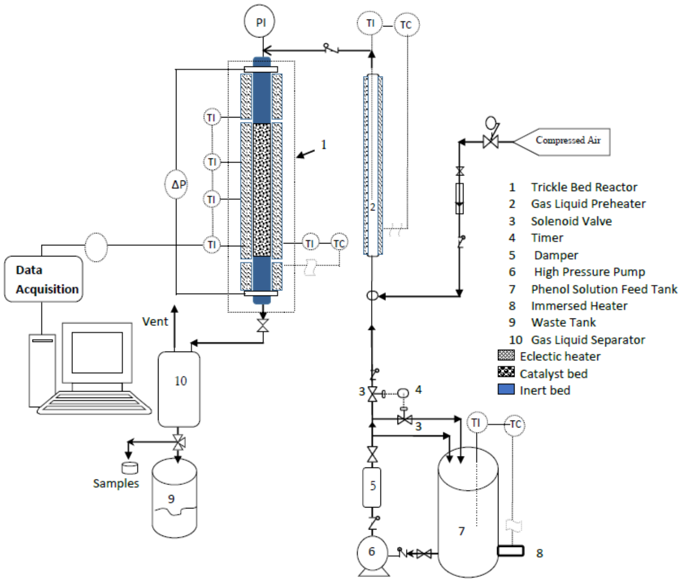
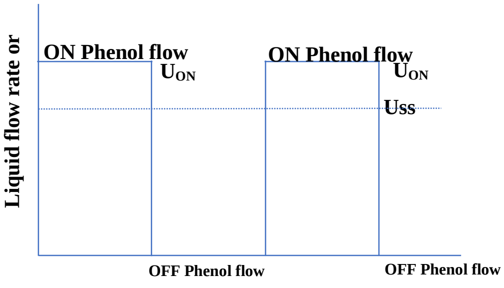
of periodic TBRs which have demonstrated that liquid flow modulation in a down flow TBRs can lead to a substantial raise in the conversion, rate of reaction and minimize liquid maldistribution, furthermore, numerous of these studies, external mass transfer resistance of the gaseous reactant is significant and the controlling step [8-29]. A few works have been dedicated to a periodic operation focused on the gas and/or liquid flow modulation and composition for the CWAO of phenol in TBRs in the last few years [23-28].They found that catalytic wet oxidation of phenol in periodic operation can significantly increases of phenol conversion towered total oxidation at 60sec cycle period and 0.5 cycle split in comparison at the steady state operation mode. [23].ON-OFF mode liquid flow modulation does not improve significantly phenol conversion but efficient mineralization of phenol (total oxidation to CO_2) occurs [24]. The proper selection of cycling parameters (cycle split and period) in CWAO of phenol by gas phase modulation, the authors found that where higher splits and cycle periods were to be highly beneficial to the catalyst activity in CWAO of phenol [25-26]. The present work aimed to investigate CWAO of phenol over a porous catalyst particle ($0.5\%Pt/\gamma\text{-}Al_2O_3$) in non-isothermal TBR for steady-state and periodic operation. The influence of key parameters on the performance of non-isothermal TBR is studied, such as periodic parameters (cycle period and split) of liquid flow modulation, furthermore space time h, bed temperature and superficial gas velocity for steady-state operation. Kinetic analysis of the studied system is also presented

2. Experimental

A pilot-plant trickle bed reactor operated in the trickle flow regime was used for steady state and periodic CWAO of phenol experiments. It is made up of a packed stainless-steel bed reactor with a diameter of 0.05 m and 1.25 m height that can be used for working at a pressure up to 4MPa, Fig. 1 Shows the experimental set up. The reactor is operated under non-isothermal conditions which were heated with external electrical heater and is linked to a controller (on-off control) that can be used to maintain the bed temperature within ±3oC of the set point temperature, four thermocouples (Type T) are used to observe the reactors' temperature zones, inserted within the reactor, and recorded continuously by data acquisition device as shown in Fig.1. Table 1, shows the properties of the bed and specifications of the catalyst and material that is being used in the experiments while Table 2 presents operating conditions investigated There are three distinct zones in the trickle bed reactor: pre-bed of inert glass particles, catalytic bed and a post-bed section of inert particles order to confirm symmetric radial liquid distribution within the reactor cross-section. The wall effect can prevented is there is a considerable reactor to particle diameter ratio = 25 [8, 19]. The liquid feed is made up by using a solution of 5 g/L of phenol (reagent grade) kept in a 100 L stainless steel storage tank and heated to a required temperature, and the tank is linked to a high pressure-metering pump (Dose pump, BALDOR FRUM DUTY, USA) that provides the phenol solution at flow rates between (0.5 – 10) L/h where liquid feed rate was the pulse can be dampened because of dosing pump which is



(a) Experimental Setup for Steady State and Unsteady State Experiment



Total Cycle Period (Time)

(b) ON-OFF Liquid Flow Modulation Arrangement

Fig. 1: (a) Experimental Setup for Steady State and Unsteady State Experiment, (b) ON-OFF Liquid Flow Modulation Arrangement

prevented by connecting a feed tank to a high pressure small stainless steel tank damper (0.04 i.d *0.35 m length). The high-pressure compressor is used for supplying oxygen found in the air which will help in delivering the gas towards the reactor after which its feed rate is calculated when it flows through calibrated rotameter The mixing and preheating of the liquid and gas streams in pre-heater is done after which it flows into the reactor at the required temperature which is then constantly observed through a K type thermocouple. The liquid outlet stream coming from the gas-liquid separator is divided into a sampling stream and a waste stream and the exiting solution (gas and liquid) from the reactor is passed through the gas-liquid separator. Pressure indicator and safety valve was placed in the gas and liquid delivery and outflow stream to prevent pressure build in .one way valve is also used to keep the flow in one direction for gas and liquid and the observation of pressure drop fluctuations during the experiment are checked through differential pressure transducer (Rosemount, model E1151 G P5523, 55T) that is linked to a data acquisition multiplexer.The liquid flow modulation was achieved for unsteady state experiments through a set of solenoid valves (CKD Nagoya Japan model 12-15G-D3A and Magnet-Schultz-Memmingen , G BPE 030 K54 D02) and timers (FoTek TDVY-M6) that are linked to a pressurized liquid delivery feed tank being utilized for switching to a steady flow, unsteady-state conditions are being conducted through ON-OFF liquid flow modulation, in which the liquid flow modulation is performed in so-called slow mode operation that is run for a time span of a few minutes.

The samples were acquired after the bed was pre-wetted and operated for various hours as this will ensure total internal wetting of the catalyst along with preheating the bed.

Table 1: Catalyst, Reactor and Material Characteristics.

Reactor Characteristics	
Reactor diameter m (I.d)	0.05
Wall Thickness m	0.005
Catalyst bed depth m	1
Pre packing depth m	0.15
Post packing depth m	0.1
Type of inert bed Glass bead mm	0.2
Catalyst Characteristics	
Active metal	0.5%Pt
Catalyst support	γ-Al_2O_3
Particle shape	Sphere
Particle diameter (cm)	0.16
Surface area(m^2/gm)	250
Pellet density(gm/Cm^3)	0.56

Table 2: Range of Operating Conditions

Operating Conditions	**CWAO**
Steady State Operation	
Inlet phenol concentration, (g/L)	5
Total Reactor Pressure, (MPa)	0.8
Equilibrium partial pressure, (MPa)	0.12-0.69
Oxygen partial pressure, (MPa)	0.168
Bed temperature, (˚C)	105-165
Liquid flow rate, (L/h)	5.8-1.4
Superficial liquid velocity (m/s)	8.34E-4 - 2.08E-4
Gas flow rate, (NL/h)	70.7-17.6
Superficial gas velocity, (m/s)	0.01- 0.0025
LHSV, (h^{-1}) Space time, (h)	1.25- 5 0.2-0.8
Unsteady State Operation	
Cycle time (period), (min)	2,9,16
Cycle split (ON flow fraction)	0.25, 0.45, 0.65

Several steady-state tests run were conducted as there was some disturbance in between each set of unsteady-state runs guarantee reproducibility of the catalyst activity in each set which otherwise liquid samples were withdrawn from the gas–liquid separator after steady state was reached at each liquid flow rate and analyzed for phenol content by a direct photometric method (UV-VV-1100, UEBO9025) and HPLC (DIONEX (UV (JYNKOTEK)/VIS160S)).

Conversion in periodic operation (unsteady-state) was evaluated by collecting concentration of a liquid sample over multiple cycles to get the time average conversion, phenol conversion was calculated according to:

$$X_{Ph} = \frac{[C_{Ph}]_0 - [C_{Ph}]_{out}}{[C_{Ph}]_0} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 1$$

$$\text{Enhancement Conversion} = \frac{\text{Average Conversion (Unsteady state)}}{\text{Conversion (Steady state)}} \ldots\ldots\ldots 2$$

All periodic experiments were initiated after the reactor had been operating at steady state. The ranges of operating conditions investigated are presented in Table 2. The feed concentrations for gas and liquid and operating conditions were chosen so as to examine both gas- and liquid-limited conditions. To compare results, the relationship between the superficial liquid velocity for steady-state operation (u_{Lss}) and during the ON cycle of periodic operation (u_{LON}) is taken into account as:-

$$U_{LON} = \frac{U_{LSS}}{S} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3$$

Where,

$$\text{Cycle Split (S)} = \frac{\text{ON Cycle Time}}{\text{Total Cycle Period}} \ldots\ldots\ldots 4$$

1. Results and discussions

3.1 Reaction Kinetics.

In present work, the kinetic model representing the experimental kinetic data of the CWAO of phenol has been the first-order reaction with respect to phenol concentration which in agreement with previous studies [1,3], TBR follows a plug flow model and a simple power law were suitable to describe the mineralization of phenol to inorganic product as:-

$$-r_{ph} = K_{ob}\, C_{ph}^{\alpha} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 5$$

$$-r_{ph} = k_o.\mathrm{EXP}\left(-\frac{E_{ob}}{RT}\right).x_{O_2}^{\beta}\, C_{ph}^{\alpha} \ldots\ldots\ldots\ldots 6$$

The conversion were analyzed to get an apparent kinetic rate (K_{ob}):

$$K_{ob} = -\left(\frac{1}{\tau}\right)\ln(1-x) \ldots\ldots\ldots\ldots\ldots\ldots\ldots 7$$

The apparent kinetic rate constant K_{ob} is obtained by plotting $-\ln(1-x)$vs. τ as shown in Fig. 2.

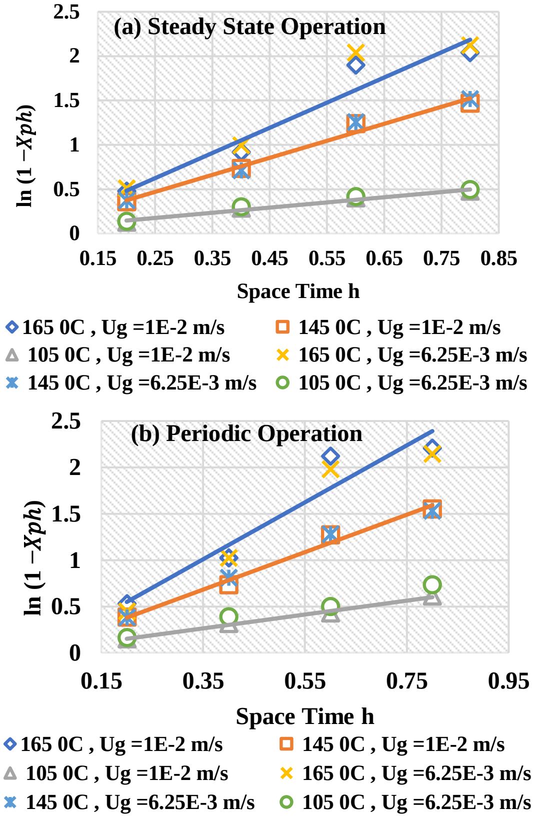


Fig. 2: Ln (1 −*Xph*) vs. Space Time for, a) Steady State Operation, b) Periodic Operation at 2 min cycle period , 0.65 cycle split.

Table 3 shows K_{ob} results for steady state and cyclic (periodic) operation at different superficial gas velocity and bed temperature, it can be noticed a certain scattering, i.e. that the $K_{ob}$was independent on the superficial gas velocity. This results emphasis the validity of the pseudo first order assumption. As observed in Table 3, it is obvious that the apparent rate constant for periodic operation is higher than that for steady state operation. For cycle period 9 min that the apparent rate constant is greater than for a 16 min cycle period, this indicates that the longer periods are not appropriate for best performance. Interestingly, a comparison detects that the apparent rate constants in periodic operation up to 9 min cycle period exceeds steady-state apparent rate constant value.

Table 3: Mean Value of Apparent Kinetic Rate

	105 °C	145 °C	165 °C
Steady State Operation	$K_{ob}\ \frac{m^3}{Kg_{catalyst}\cdot h}$		
	0.581	1.921	2.833
Periodic Operation	$K_{ob}\ \frac{m^3}{Kg_{catalyst}\cdot h}$		
2 min cycle, 0.25 split	1.0777	3.152	15.216
2 min cycle, 0.45 split	0.956	2.384	3.0315
2 min cycle, 0.65 split	0.924	2.0121	3.027
9 min cycle, 0.25 split	1.3866	4.511	16.751
9 min cycle, 0.45 split	1.235	3.115	3.564
9 min cycle, 0.65 split	1.1432	2.602	2.775
16 min cycle, 0.25 split	0.5516	1.851	2.465
16 min cycle, 0.45 split	0.462	1.377	1.679
16 min cycle, 0.65 split	0.368	0.991	1.136

The activation energy (Eo$_b$) of phenol oxidation was determined by Arrhenius plot, and liner regression analysis of the data shown in Table 4. Comparison with the activation energy obtained for steady state operating, an efficient mineralization occurs for phenol (total oxidation to CO_2) during periodic operation. Our results are in good agreement with the findings of Joglekar et al. [29]; Atwater et al. [30] Hamoudi et al. [31] and Luna et al. [32]. Furthermore, for periodic operation, activation energy (Eob) varied with the cycle period and split due to the variation in the reaction mechanism from a kinetically controlled reaction to a gas-phase controlled reaction also the higher values of activation energy (Eo$_b$) especially at 2 min, 0.25 split and 9 min, 0.25 split indicate that the a partial oxidation of phenol occurs to intermediates compounds of low molecular weight carboxylic acids. The present trends are in accordance with the findings of Castellari and Haure [13] and Urseanu et al. [16] for their reaction system

Table 4: Activation Energy (E_{ob}) (KJ/mol)

Steady State Operation		
Regression coefficient R		E_{ob} **(kJ/mol)**
0.9964		**36.858**
Periodic Operation		
Cycle Period, Split	**R**	E_{ob} **(KJ/mol)**
2 min, 0.25 split	0.892	56.27
2 min, 0.45 split	0.9901	27.097
2 min, 0.65 split	0.997	26.931
9 min, 0.25 split	0.935	53.935
9 min, 0.45 split	0.967	25.38
9 min, 0.65 split	0.946	21.517
16 min, 0.25 split	0.986	35.29
16 min, 0.45 split	0.976	30.704
16 min, 0.65 split	0.965	27.032

3.2. Effect of Operating Conditions on Performance of Trickle Bed Reactor.

3.2.1. CWAO of Phenol - Steady State Operation

Fig. 3 and 4 give the indication of steady state phenol conversion for different operating conditions at various space time ,superficial gas velocity and bed temperature . As can be seen in these Figs., phenol conversion increases from 12..to 39%as space time increased from 0.2 to 0.8h at temperature = 105 °C for the case of no phase change, while phenol conversion increases from 37.5 % to 87% as space time increased from 0.2 to 0.8h at temperature = 165 °C with considering phase change . This suggests a percentage increase in phenol conversion = 123% When the reactor operated from no phase change to phase change. These results attributed to the fact that the catalyst surface is partially wetted and the reactor operated under gas limited conditions where the diffusion fluxes $\gamma > 1$ as shown in Table 5, The catalyst pores which are internally filled with liquid, the dry partially surface exposed to the gas phase for longer liquid residence time thus water evaporation and phenol removal more suitable. The portion of liquid inside the pores of the catalyst pellet has greater opportunity to transfer to the gas phase from the dry catalyst surface, furthermore the capillary driving force which build up for the liquid diffusing from the wet part catalyst surface into the catalyst pores. Accordingly, further reactant (phenol) gets within the catalyst and reaches the catalyst's active sites. As can be seen in Fig. 5 that partial wetting and phase change have positive effect on the catalyst performance. However, according to this result, as the reactor operates under partial wetting conditions, outlet phenol concentration decreased (i.e., incresed phenol conversions) in all conditions studied. Direct gas - solid mass transfer will further diminish the weak influence of gas and liquid mass transfer limitations. Present results agree well with the findings of, Eftaxias et al.[3]; Stuber et al.[33]; Guo and AL-Dahhan, [34] and Massa et al., [24]. The effect of superficial gas velocity on the phenol conversion is shown in Fig (4). It seems that the slight effect of superficial gas velocity, can be explained by the kinetically controlled, absence of external transport limitation, and by its balanced influences on mass transfer and on vaporization effect at elevated temperature. These results agree well with findings of Guo and AL-Dahhan, [34] and Goto and Smith[38].

Table 5: Values of Diffusion Fluxes (γ)

0.8 MPa, $C_{ph0} = 5000$ ppm (0.05311 kmol/m^3)				
T °C	O_2 Solubility ^{a} kmol/m^3	Diffusion Coefficient ^{b} m/s		γ ^{c}
		Phenol	O_2	
105	3.461E-05	4.416E-09	1.417E-08	68.291
145	3.503E-05	6.957E-09	2.233E-08	67.466
165	3.765E-05	8.385E-09	2.691E-08	62.768

a O_2 Solubility from Henry's law constant by Crammer correlation [35]

b Diffusion coefficient calculated from Wilke–Chang correlation [36]

c According to the Beaudry et al.[37] and Khadilkar et al.[19] criterion which was particularly useful to diagnose the gas and liquid reactant limitation

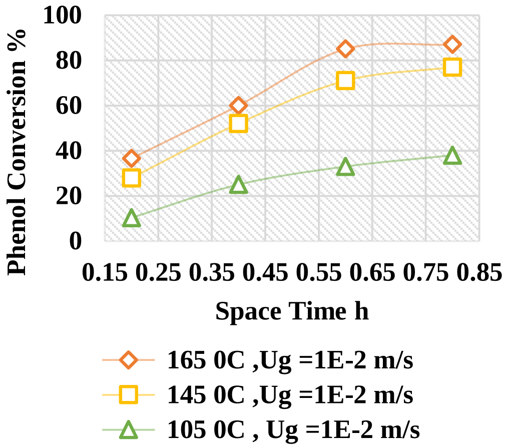


Fig .3: Conversion vs. Space Time at different bed Temperature and Superficial Gas Velocity [phase changes are considered in 165 and 145 oC].

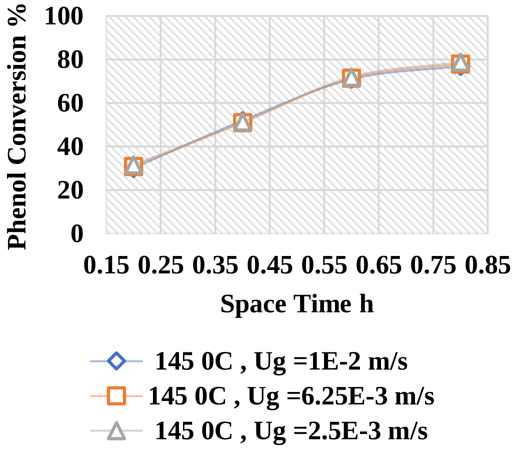


Fig .4: Conversion vs. Space Time at different bed Temperature and Superficial Gas Velocity [phase changes are considered between space time 0.6-0.8h].

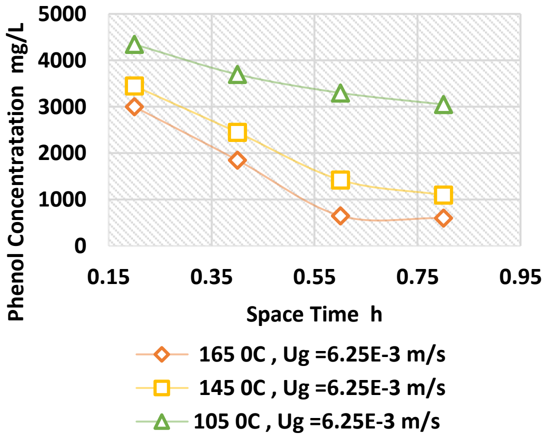


Fig. 5: Phenol Concentration vs. Space Time at different bed Temperature and Superficial Gas Velocity =6.25E-3 m/s.

The increased phenol conversion at higher temperature is also shown in Fig. 3 and 4, a temperature increment of 60 ^{o}C resulted in an evident enhancement (up to 88.7%) of the phenol conversion, it is evident that at high temperature and space time, resulting increasing driving force and the equilibrium water vapor pressure that enhance phase change and enhancing the phenol conversion .This is attributed to the fact that the system is under chemical kinetic control. These results confirm the opinion of Eftaxias et al.[39]; Watson and Harold [7].At low bed temperature, water vapor pressure is small and heat release because of the reaction dominates in the heat balance, so that the producing temperature increased and this effect was much higher for elevated temperature at 145 and 165 ^{0}C where phase change more pronounced .For space time 0.6h, superficial gas velocity 0.0025 m/s bed temperature 165^{o}C results phenol conversions 87.6% with a temperature rise of 7 ^{o}C is attained, the equilibrium water vapor pressure jumps from 0.696 to 0.826 MPa, which becomes the evaporation phenomenon becomes pronounced.

3.2.2. Periodic operation (Unsteady state).

The influence of cycle split on phenol time average conversion and performance enhancement at various cycle periods is shown in Fig. 6, it seems that phenol time average conversion and performance enhancement was improved and the observed improvement in conversion reaches as much as 14.94- 84.68% over the steady state(S=1) at the same space time at cycle split of S=0.25. The enhancement reached 14.94% at 0.8h space time, 165 ^{o}C bed temperature, 0.01 m/s superficial gas velocity with time average conversion 100% while 84.68% performance enhancement reached at 0.2h space time, 105^{o}C bed temperature, 0.0025 m/s superficial gas velocity. In ON–OFF flow modulation, cyclic renewal of liquid on catalyst pellet surface and negligible liquid film resistance in OFF cycle period. Performance enhancement is achievable by increasing gaseous reactant supply onto the catalyst; gas-to-liquid ratio access times was varied with vary of cycle split at a constant space time and/or mean liquid mass velocity. Our results agree well with the findings of Lange et al. [20], Turco et al. [22] and Liu et al. [18].The effect of the total cycle period on phenol time average conversion and performance enhancement at various cycle split can be noticed in Fig. 7, where the conversion enhancement seems to increase with cycle period up to 9 min period, after which it drops below steady state values up to 30.36-54.04% at higher cycle period. Similar findings were reported by Massa et al.[23], Lange et al. [20] and Haure et al. [8] in their reaction systems. In the period of cut off liquid flow, the reaction takes place between the liquid holdup and the gas phase (air), also elevated bed temperatures of the heat catalytic oxidation reaction reduces by modulation of the liquid flow [7]. Gas phase reaction occur due to the evaporation of the liquid phase under these conditions. Different activation energies obtained due to the change in the reaction mechanism from a kinetically controlled reaction to a gas phase controlled reaction .Partial dry of catalyst surface was observed after time of exposure to the gas phase, the reaction temperature reaches a maximum as the holdup is depleted and evaporation phenomenon becomes pronounced. Temperature rise during the ON-OFF cycle is s shown in Fig. 8, for optimum cycle period of 9 min and various cycle split with and without considering phase changes. It is obvious that a temperature rise of 7 **^{o}C** is attained at a cycle split = 0.5 while it attained 16 ^{o}C at a cycle split = 0.25, under these conditions equilibrium water vapor pressure increased from 0.499 to 0.633 MPa, and vaporization may occur. The sudden increased in temperature observed after the OFF time period of exposure to the gas phase only could be attributed to the gas phase reaction over a dry catalyst. The higher temperature amplitude attended is 20 ^{o}C when the initial bed temperature 165 ^{o}C at space time 0.8h, optimum cycle period of 9 min, cycle split 0.25

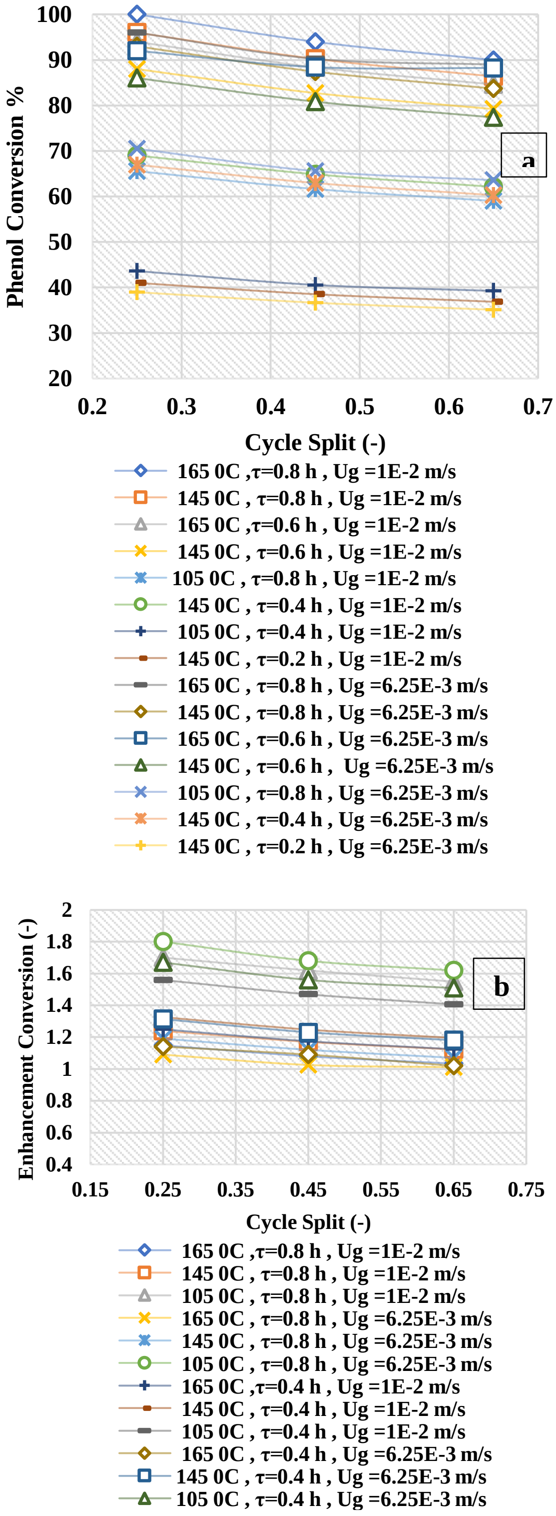


Fig. 6: Enhancement conversion vs. cycle split at 9min cycle period at different bed temperature and superficial gas velocity, (a) phenol conversion, and (b) enhancement conversion.

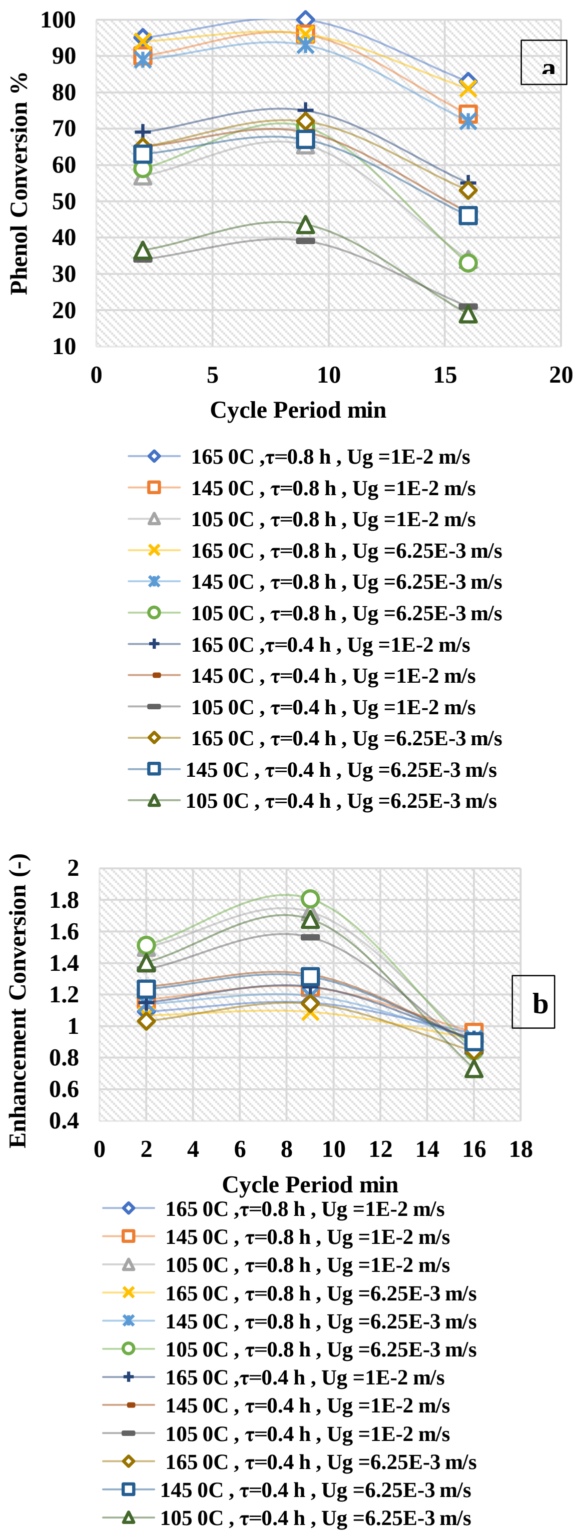


Fig. 7: Enhancement conversion vs. cycle period at 0.25 cycle split as s function of bed temperature and superficial gas velocity, (a) phenol conversion, and (b) enhancement conversion

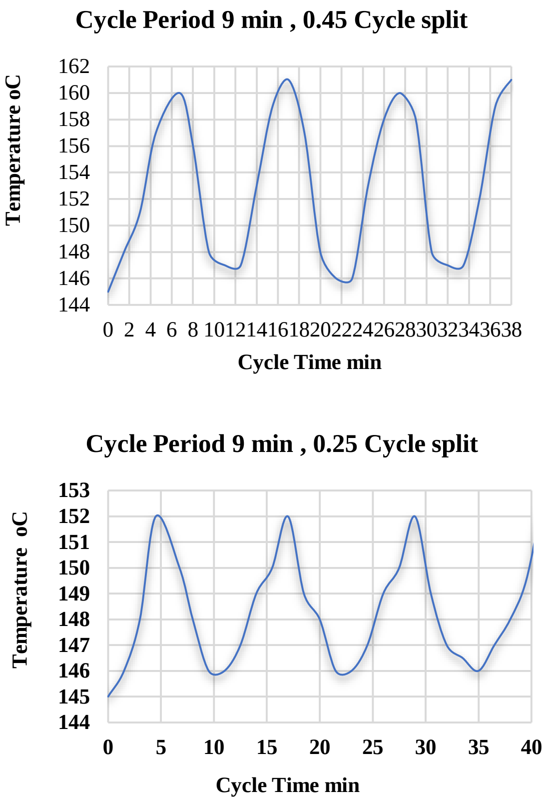


Fig. 8: Temperature profiles for different cycling conditions at space time 0.8h and initial bed temperature 145 °C.

4. Conclusion

The present study aimed to investigate the effect of periodic operation on the process performance of a catalytic trickle bed reactor which extensively used in petroleum and petrochemical industries.

In this work, phenol is oxidized in a trickle bed reactor using ON-OFF mode of liquid flow modulation over 0.5%Pt/γ-Al_2O_3 catalyst. Experimental results showed that the performance of CWAO of phenol has been significantly enhanced up to 14.94- 84.68% under periodic operation to a maximum value at 0.25 cycle split and 9min cycle period, while it drops to 30.36-54.04% lower steady state value at higher cycle period and split under identical operating conditions with steady state operation. It was shown that temperature effects of an exothermic reaction, cyclic wetting of catalyst surface are strongly influenced by modulation parameters such as cycle period and split. The higher temperature amplitude attended is 20 °C when the initial bed temperature 165 °C at space time 0.8h, optimum cycle period of 9 min, cycle split 0.25. For periodic operation, activation energy (E_{ob}) varied with the cycle period and cycle split due to the change in the reaction mechanism from a kinetically reaction to a gas phase reaction.

Acknowledgment

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Notations

C	Concentration	$kmol/m^3$
E_{ob}	Activation energy	kJ/mol
K_{ob}	Observed rate constant	$kg_{catalyst}$ $/.m^{3.}h$
k_o	Frequency factor (case dependent units)	
r	Reaction rate	$kmol/kg_{cat}.h$
T	Temperature	^0C
U_0	Initial Liquid velocity	m/s
u_{Lss}	Superficial Liquid velocity for steady-state operation	m/s
u_{LON}	Superficial Liquid velocity during the ON cycle of periodic operation	m/s
x	Conversion	(-)

Greek Symbols:

α	Phenol order	(-)
β	Oxygen order	(-)
γ	Reactant limitation criteria	(-)
ν	Stoichiometric coefficients of oxygen	(-)
τ	Space time	h

Subscripts:

O_2	Oxygen
out	Output
ob	Observed

Ph	Phenol
0	initial

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