ASSIGNMENT 2

CHEMICAL REACTION ENGINEERING

METHOD OF INITIAL RATES

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QUESTION

Method of Initial Rates

	Π = 1		Π = 3		Π = 4		Π = 7	
	X	W/F	X	W/F	X	W/F	X	W/F
	0.118	0.2	0.14	0.2	0.14	0.2	0.112	0.2
	0.196	0.4	0.2	0.4	0.196	0.4	0.163	0.4
	0.292	0.6	0.25	0.6	0.235	0.6	0.194	0.6
	0.339	0.88	0.286	0.88	0.271	0.88	0.214	0.88
	0.446	1.53	0.352	1.6	0.32	1.6	0.254	1.6
	0.454	1.6						
	0.524	2.66						
	0.59	4.22						
	0.6	4.54						
	$X = a \tanh (bW/F)$							
a=								
b =								
$r_0 = dx/d(W/F)$ at $W/F = 0$ =								

Plot r_0 vs Π and deduce the rate controlling step.
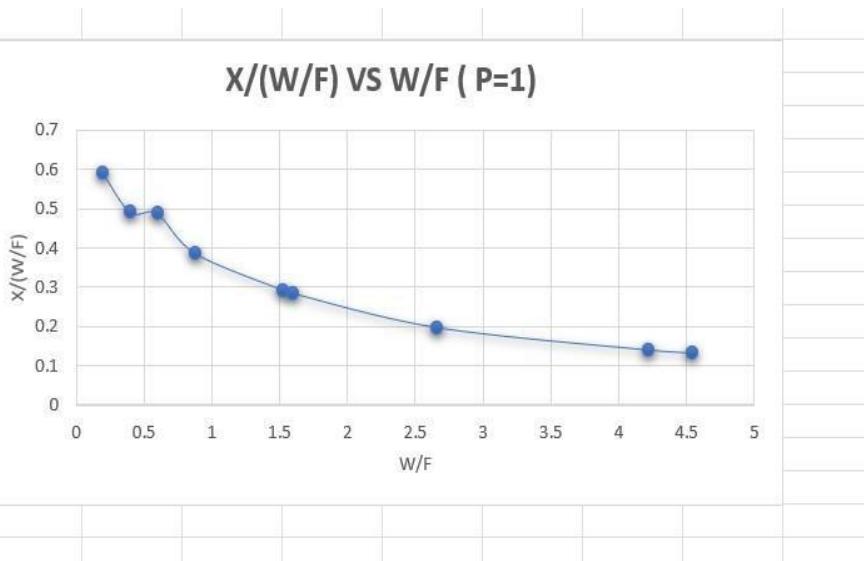
SOLUTION

METHOD 1

# BY THE INTERCEPT OF X/(W/F) vs W/F WHICH WILL GIVE VALUE OF INITIAL RATE
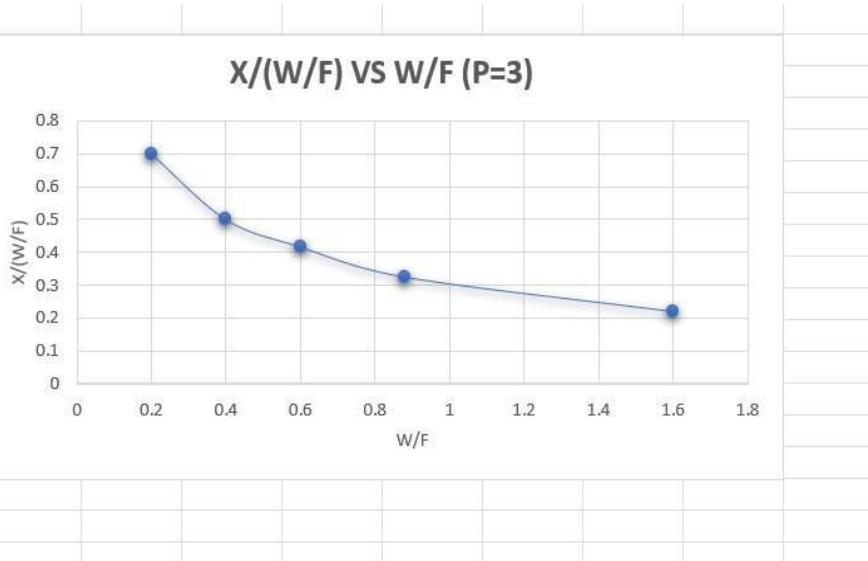
Pressure = 1 bar

P = 1		
W/F	X	X/(W/F)
0	0	
0.2	0.118	0.59
0.4	0.196	0.49
0.6	0.292	0.486667
0.88	0.339	0.385227
1.53	0.446	0.291503
1.6	0.454	0.28375
2.66	0.524	0.196992
4.22	0.59	0.13981
4.54	0.6	0.132159
INTERCEPT		0.69
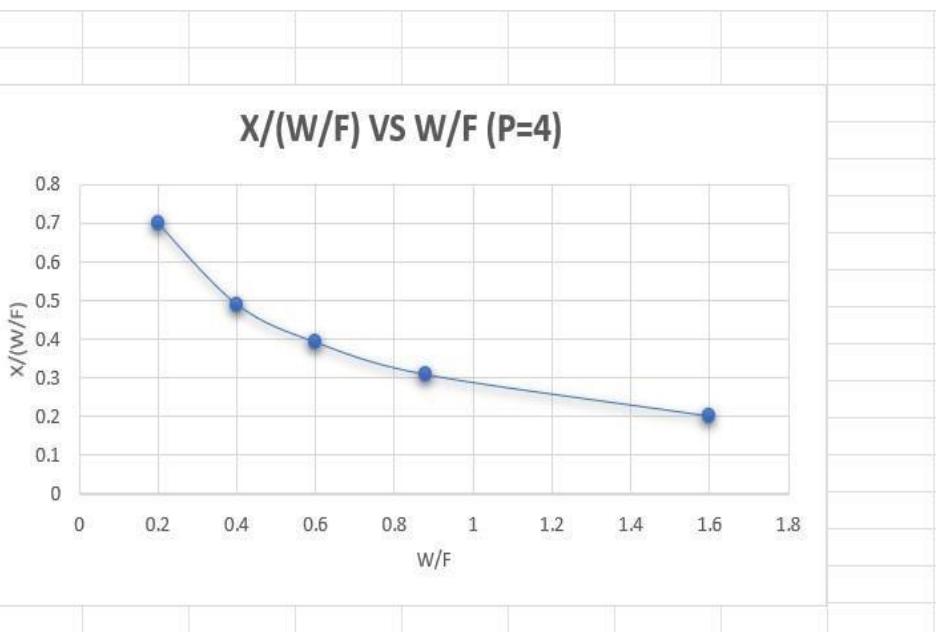
Pressure = 3 bar

P = 3		
W/F	X	X/(W/F)
0	0	
0.2	0.14	0.7
0.4	0.2	0.5
0.6	0.25	0.416667
0.88	0.286	0.325
1.6	0.352	0.22
INTERCEPT		0.9

X/(W/F) VS W/F (P=3)
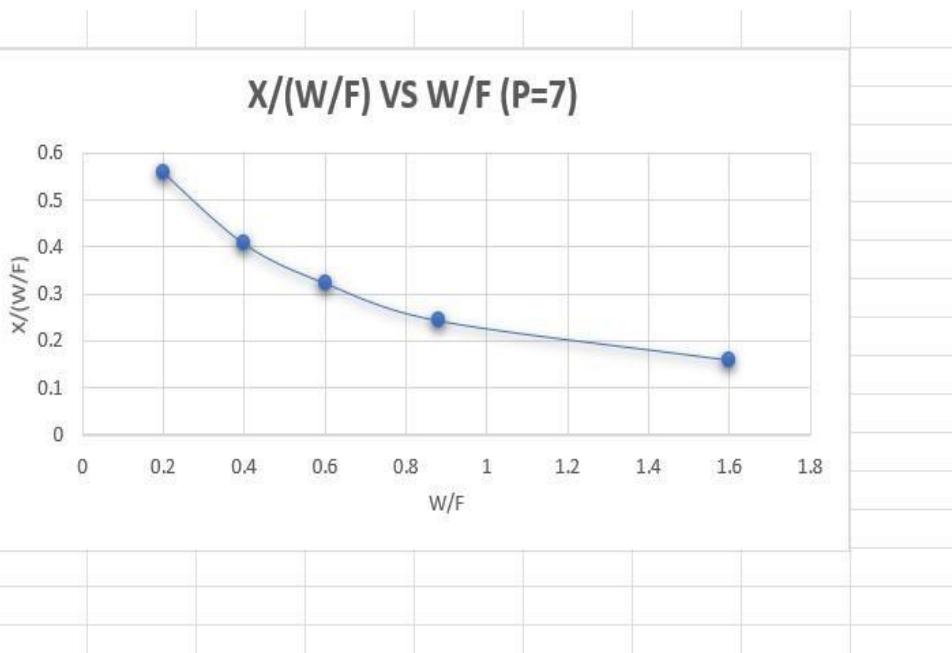
Pressure = 4 bar

P = 4		
W/F	X	X/(W/F)
0	0	
0.2	0.14	0.7
0.4	0.196	0.49
0.6	0.235	0.391667
0.88	0.271	0.307955
1.6	0.32	0.2
INTERCEPT		0.91

X/(W/F) VS W/F (P=4)
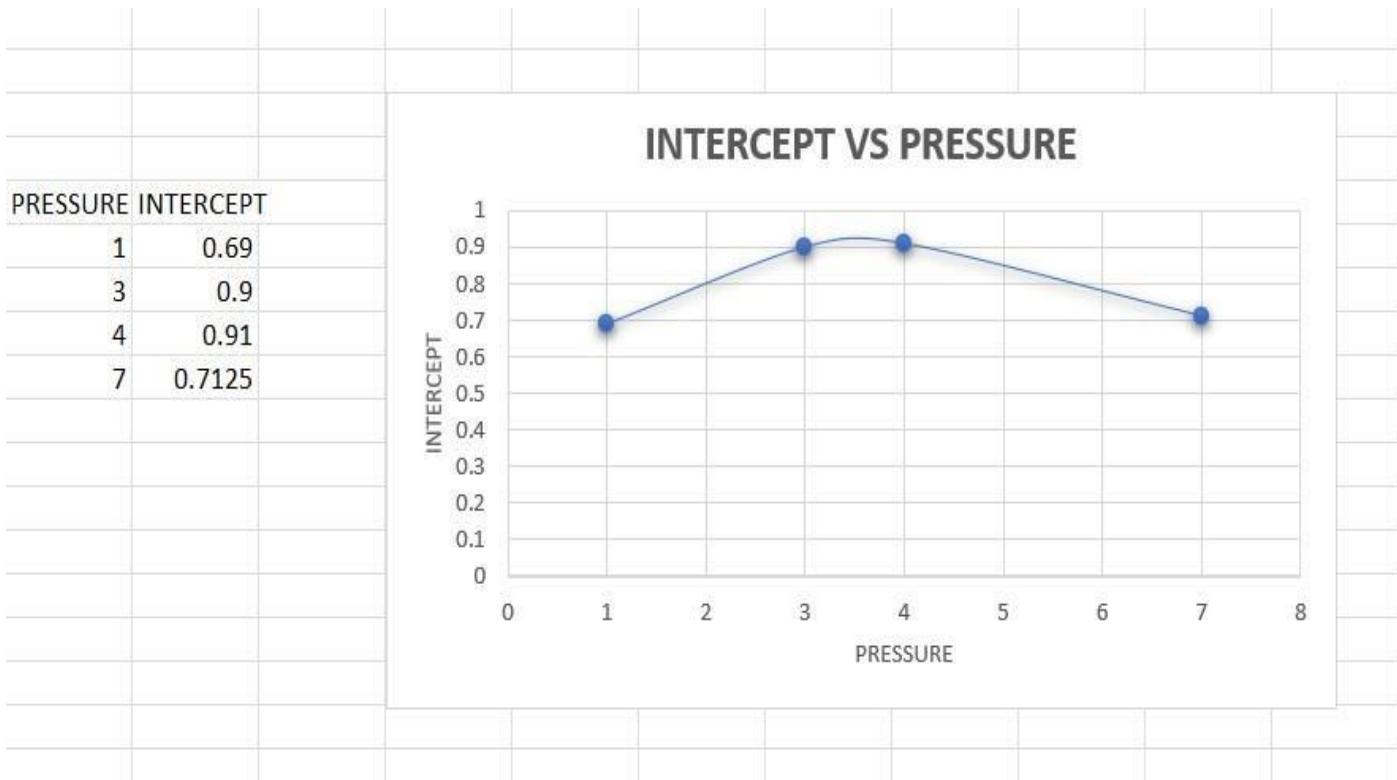
Pressure = 7 bar

P = 7		
W/F	X	X/(W/F)
0	0	
0.2	0.112	0.56
0.4	0.163	0.4075
0.6	0.194	0.323333
0.88	0.214	0.243182
1.6	0.254	0.15875
INTERCEPT		0.7125

X/(W/F) VS W/F (P=7)

Intercept(rA0) vs Pressure

| PRESSURE	INTERCEPT
1	0.69
3	0.9
4	0.91
7	0.7125

INTERCEPT VS PRESSURE
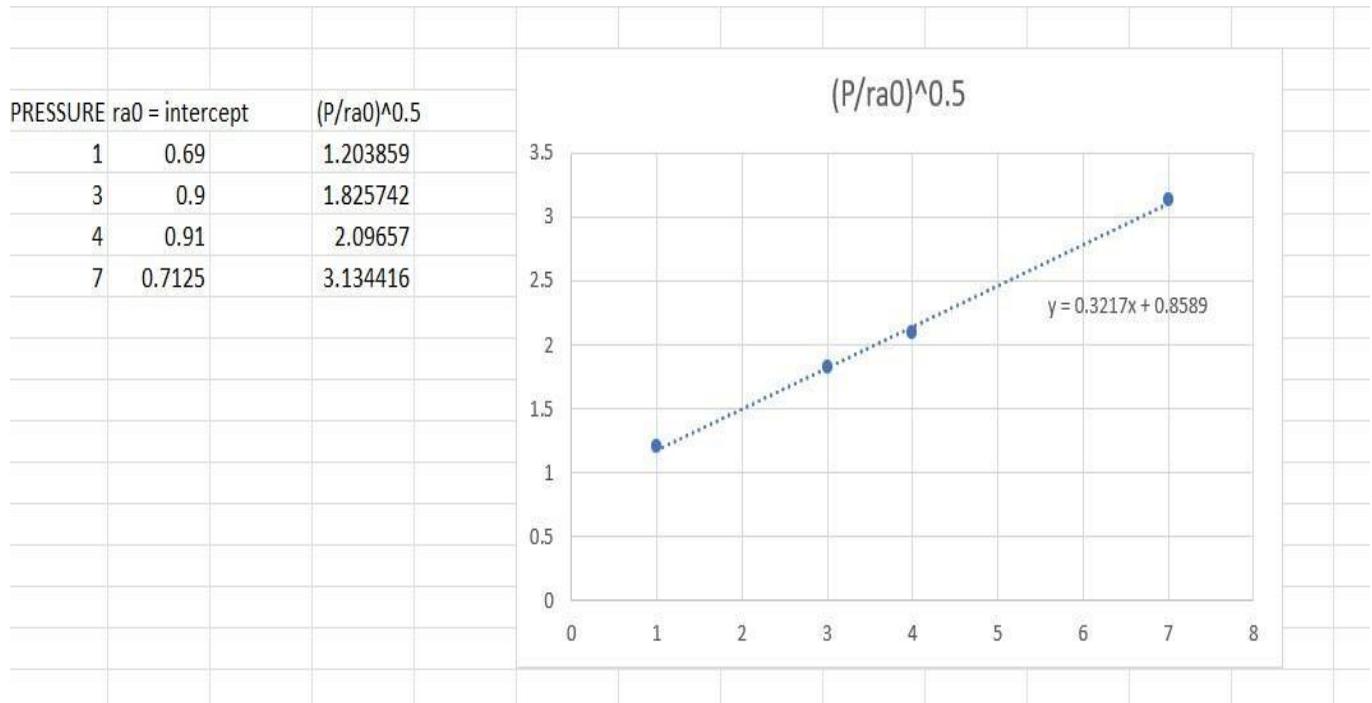
CONCLUSION:

From the graph of initial rate versus total pressure, it is observed that the reaction rate first increases with pressure but later levels off and becomes nearly constant at higher pressures. This trend suggests that the **Chemical Reaction Step Controls** the rate, not adsorption or diffusion.

METHOD 2

BY THE FITTING OF X AND W/F IN EMPIRICAL EQUATIONS

For calculating values of "a" and "b" graph of $(P/rA0)^{0.5}$ vs Pressure

PRESSURE	ra0 = intercept	$(P/ra0)^{0.5}$
1	0.69	1.203859
3	0.9	1.825742
4	0.91	2.09657
7	0.7125	3.134416

$(P/ra0)^{0.5}$

$y = 0.3217x + 0.8589$

From Graph
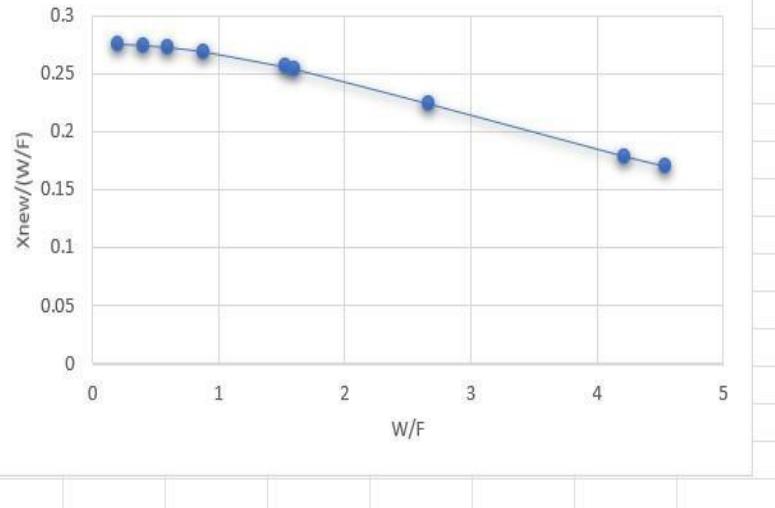
Intercept = a = 0.8589

Slope = b = 0.3217

Pressure = 1 bar

P = 1				
W/F	X	X/(W/F)	Xnew=a*tanh(b*W/F)	Xnew/(W/F)
0	0			
0.2	0.118	0.59	0.055185498	0.275927
0.4	0.196	0.49	0.109917231	0.274793
0.6	0.292	0.486667	0.163756238	0.272927
0.88	0.339	0.385227	0.236857196	0.269156
1.53	0.446	0.291503	0.391625411	0.255964
1.6	0.454	0.28375	0.406787604	0.254242
2.66	0.524	0.196992	0.596116941	0.224104
4.22	0.59	0.13981	0.752249696	0.178258
4.54	0.6	0.132159	0.771080187	0.169841
INTERCEPT(NEW)		0.27707		
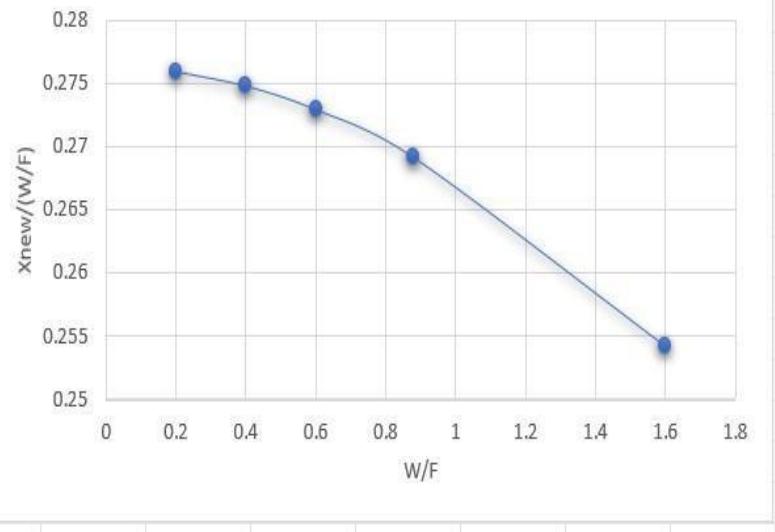
Xnew/(W/F) vs W/F (P=1)

Pressure = 3 bar
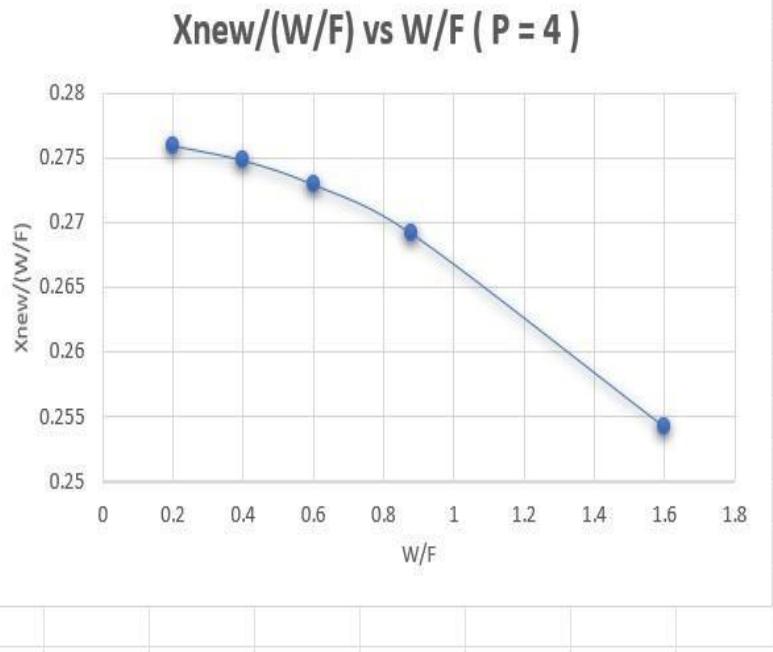
P = 3				
W/F	X	X/(W/F)	Xnew=a*tanh(b*W/F)	Xnew/(W/F)
0	0			
0.2	0.14	0.7	0.055185498	0.275927
0.4	0.2	0.5	0.109917231	0.274793
0.6	0.25	0.416667	0.163756238	0.272927
0.88	0.286	0.325	0.236857196	0.269156
1.6	0.352	0.22	0.406787604	0.254242
INTERCEPT		0.27707		

Xnew/(W/F) vs W/F (P = 3)

Pressure = 4 bar

W/F	X	X/(W/F)	Xnew=a*tanh(b*W/F)	Xnew/(W/F)
P = 4				
0	0			
0.2	0.14	0.7	0.055185498	0.275927
0.4	0.196	0.49	0.109917231	0.274793
0.6	0.235	0.391667	0.163756238	0.272927
0.88	0.271	0.307955	0.236857196	0.269156
1.6	0.32	0.2	0.406787604	0.254242
INTERCEPT		0.27707		
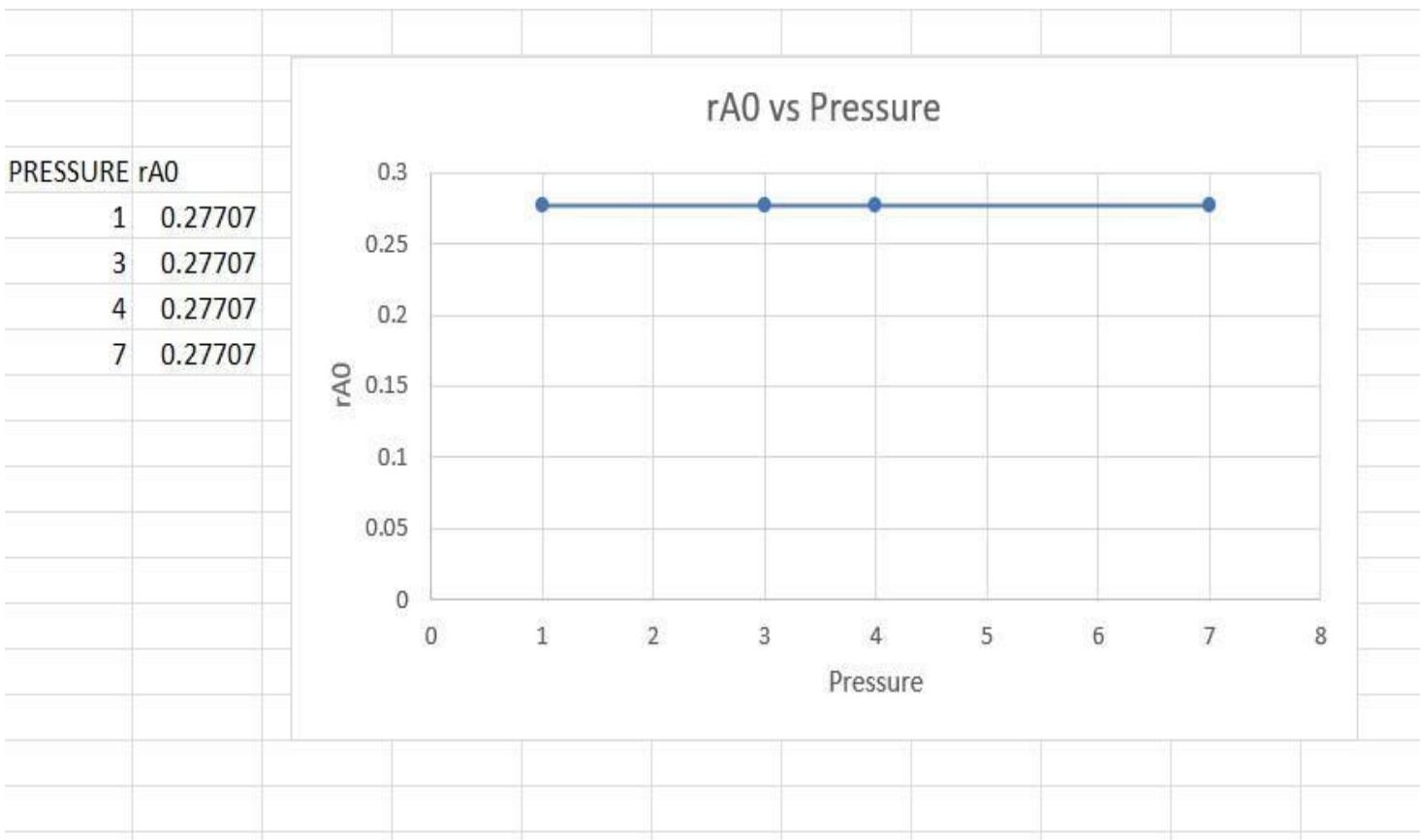
Pressure = 7 bar

W/F	X	X/(W/F)	Xnew=a*tanh(b*W/F)	Xnew/(W/F)
P = 7				
0	0			
0.2	0.112	0.56	0.055185498	0.275927
0.4	0.163	0.4075	0.109917231	0.274793
0.6	0.194	0.323333	0.163756238	0.272927
0.88	0.214	0.243182	0.236857196	0.269156
1.6	0.254	0.15875	0.406787604	0.254242
INTERCEPT		0.27707		

rA0 vs Pressure

PRESSURE	rA0
1	0.27707
3	0.27707
4	0.27707
7	0.27707

rA0 vs Pressure

CONCLUSION:

From the plot of versus pressure, the calculated values are and. Additionally, the curve of versus pressure appears as a straight horizontal line, indicating that remains constant with changing pressure. This behavior suggests that **Desorption Step** is the **Rate-Controlling** step in the reaction.