Computational Fluid Dynamic Simulation of an Industrial Ethylene Decholride Thermal Reactor

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Abstract: *In the coming decades, polyvinyl chloride (PVC) is considered as the common plastics in petrochemical industries due to its high potential application. To make PVC's, monomers were produced firstly which is called vinyl chloride(VCM). This process is done in the ethylene dichloride thermal (EDC) cracking reactor within the temperature profile range of 680-758 ° K and the pressure drop of 25*105 Pascal. The objectives of this comprehensive study is to simulate 2D of thermal cracking reactor with FLUENT software and compare with an industrial reactor to obtain an optimum EDC conversion factor. Furthermore, the crucial parameters and their profound impact on the calculation of EDC conversion factor were taken into the consideration to spouse the importance of each parameter. Consequently, EDC conversion factor with the percentage of 52.69 has a good agreement with industrial data.*

Keywords: *Polyvinyl Chloride, Vinyl Chloride, Ethylene Dichloride Thermal, Conversion Factor, FLUENT Software*

1. INTRODUCTION

Smart manufacturing (SM) is considered to those performances which are utilized and performed the intelligence of manufacturing provide sufficient production chains to obtain to the dramatic increase of current operational occasions. Manufacturing intelligence (MI) entails two different segments; the ubiquitous and affordable application of web-based technologies and pervasive administration of data gathering and its analysis, modelling and simulation procedures and subsequently the optimization processes to achieve a balance between components. To obtain the proper utilization of manufacturing intelligence in an industrial purpose, understanding of real-time circumstances, reasonable phenomena, pre- planned and accurate planning, and satisfying management of all steps of the manufacturing processing are urgently needed to address the current situation[1-5]. The appropriate designation and analytical simulation of thermal cracking reactors due to the complexity of chemical reactions among industrial procedures and the phenomenon of heating transfer in the furnace layers are the main concerns of petrochemical industries which they are effectively elaborated by numerous research activities to address the current industrial problems. In the coming decades, the administration of computational fluid dynamics (CFD) is widely popularized to facilitate the simulation of processing modulus like thermal cracking reactors and other equipment schematically to estimate the parameters such as velocity, and mass volume of transferred gas properly in the laboratory circumstances. Hence, these pre-planned analytical simulations which are principally based on the precious correlations enables engineers and industries to virtually eliminate the squander vast sums of money. Furthermore, due to the enhancement of computing sciences power in the modelling of dynamics fluid and processing simulations; in respect of the way, CFD modelling would enable engineers to simulate the compositional model entail both chemical and physical procedures with more detailed representatives of reactor geometry. Therefore, CFD modelling is considered as the comprehensive technique to appropriately deal with the complexities of boundary conditions and geometry characteristics. In addition, CFD modelling gives engineers the chance to modify the designation parametric values more flexible. Ethylene is one of the main building blocks in the petrochemical industry due to its high potential reactivity to make resins, fibres and plastics. Among numerous processes in petrochemical industries to make ethylene, ethane, naphtha, and propane

thermal cracking procedures are the most common techniques which they are more affordable and preferable by petrochemical companies[5-9].

1.1. Steady State Modelling And Steady State Optimization

Shahrokhi and Nejati (2002) firstly proposed an extensive 1D steady state model of thermal cracking processes to distinguish the profile of gas temperatures alteration on the schematic reaction between molecules. Since then, Zhang, et., al. (2007) conducted an investigation into the 3D model of simulating the EDC reactors by the utilization of CFD methodologies. In this study, the profound impact of gas burners position in the firebox were taken into consideration regarding the performances of processing design goals[10-15].

1.2. Dynamic Modelling and Dynamic Optimization

Ghashghaee and Karimzadeh (2007) concentrated their insights into the dynamic modelling

of thermal cracking in the furnaces that were capable to estimate the unsteady-state crackers condition during start-up steps. Their proposed model consisted of four substantial mathematical model as convectional heat transfer model, firebox model, tube skin model, and tubular coil model. Thereby, selection of optimum Dynamic solution is illustrated as the best preferable technology to modify the current fluctuations.

1.3. Tube Geometry and Meshing

Mesh quality is one of the most substantial issue for the proper and best estimable CFD simulation and modelling procedures, i.e., a mesh with low quality needs the most robust CFD solver and subsequently accurate more computational processes to provide the best sustainable solutions. In the EDC procedures, the segments which are occupied with processing fluid in the furnace are called coils that are located in the horizontal position. The arrangement of coils in an industrial furnace are schematically depicted in figure 1. As it is evident in figure 1, the produced heat is transferred by the coils in terms of radiation of convection models.
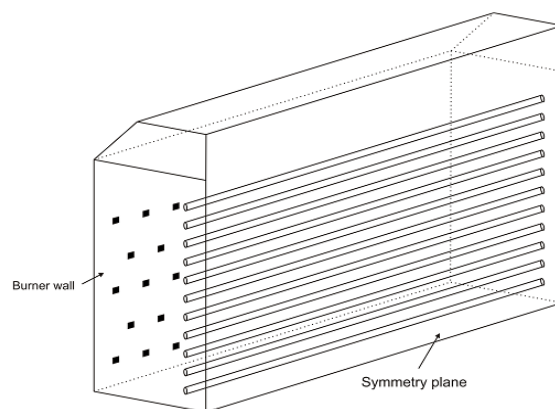

Figure1. *Arrangement of Horizontal Coils in The Furnace*

By using the equation 1, it is evident that from the EDC thermal cracking, vinyl chloride (VCM) and hydrochloric acid are produced. The major section of a thermal cracking unit is those section which cracking procedures are occurred in; in respect of the way, coils which are arranged in the furnace with a specific order. Thermal cracking furnaces are entailed radial and convectional areas. In addition, in convectional area used for the heating processes and evaporated the input feeds. The schematic of EDC thermal cracking furnace to change EDC to VCM is shown in figure 2.

$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl \tag{1}$$

Although, there are numerous studies are widely reported in literature to emphasize the considerable influence of CFD procedures in the thermal cracking reactors, in this comprehensive simulations, we try to propose an analytical EDC thermal cracking in an industrial furnace and qualify the suggested model to virtually eliminate the unnecessary expenditures. Moreover, the mathematical model would provide holistic by improving cracking reaction and increasing inside temperature of reactor, so that the conversion factor will be increased and subsequently the coke settling in the sidewall of the coil will be increased.
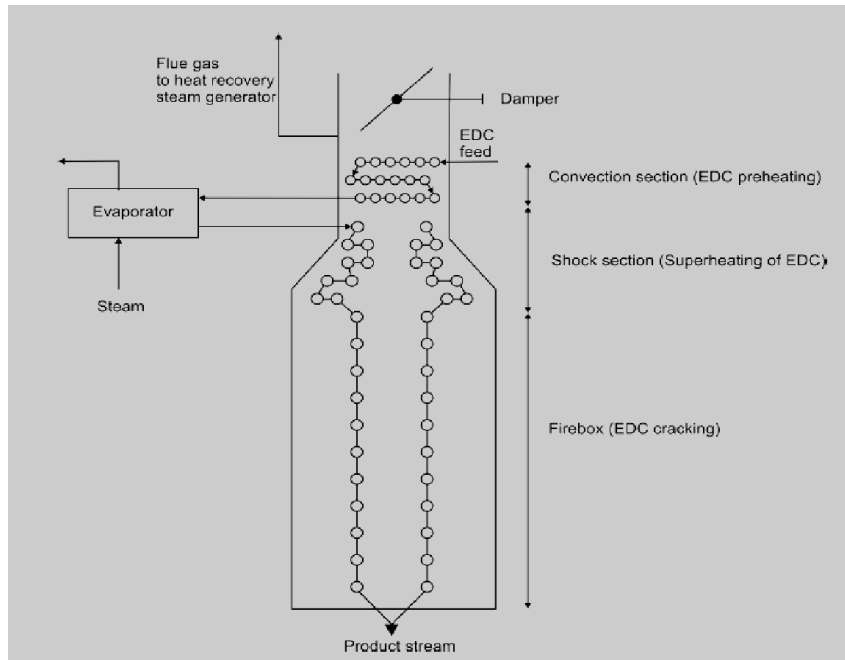
Figure2. *Schematic of EDC thermal cracking furnace to change EDC to VCM*

2. SIMULATION PROCEDURES

2.1. Governing Equations

The assumptions which are used to calculate the following equations are described in figure 3.
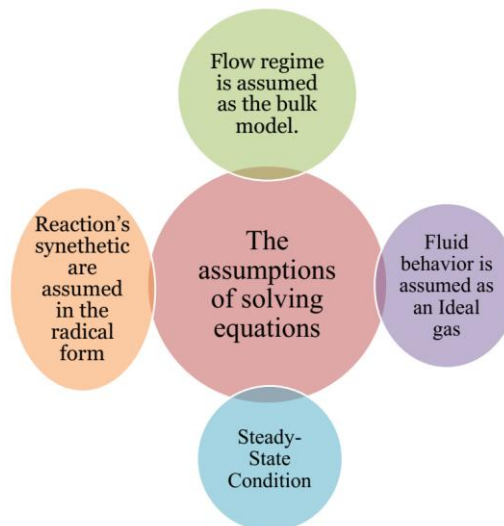

Figure3. *Required Assumptions in the Correlations*

The considered element in the length of coil which is used in mass balance equation is depicted in figure 4. So the mass balance for all the participants in the equation is according to the equation 2.

$$\frac{dF_i}{dZ} = \sum_{j=1}^{NR} \gamma_{ij} . r_j(z). M_{Wi}(z). \frac{\pi \times D_i^2}{4} \tag{2}$$

Where γ_{ij} is the stoqumeteric factor for each component and r_j is the number of each reaction which the reaction's component are described in table 1 and 2.

Figure4. *Considered element in the length of coil*

Table1. *Reaction's component (Molecule Components)*

1,2-dichoroethane	EDC
Vinyl-chloride	VCM
hydrogen chloride	HCl
Tri-chloro-methane	CHCl3
Tetra-chloro-methane	CCl4
Ethyl-chloride	EC
1,1-dichloroethane	1,1
1,1,2-trichlorothane	1,1,2
1,1,1,2,Tetrachloroethane	1,1,1,2
cis-/trans-di-chloro-ethyl	Di
trichloroethylene	Tri
1-/2-chloroprene	CP
acetylene	C_2H_2
benzene	C_6H_6
3,4- di-chloro-butane	$C_4H_6Cl_2$
Soot/coke	C

Table2. *Reaction's component (Radical Components)*

Cl*	R1
$CH_2Cl-CH_2*/CH_3-CHCl*$	R2
$CH_2Cl-CHCl*$	R3
$CHCl_2-CH_2*$	R4
$CHCl=CH*/CH_2=CCl*$	R5
$CH_2Cl-CCl_2*/CHCl_2-CHCl*$	R6
$CHCl_2-CCl_2*/CCl_3-CHCl*$	R7
CCl_3*	R8

In the simulating processes with Fluent software, the equation for mass balance conditions is as equation 3;

$$\frac{\partial(\rho y_i)}{\partial t} + \frac{\partial(\rho u_i y_i)}{\partial x_i} = -\frac{\partial J_i}{\partial x_i} + R_i + S_i \tag{3}$$

Where ρ is Density, t is the period time, u_i is the potential energy, J_i is the diffusion term which demonstrated as the infiltration term and it doesn't utilized in the simulation processes, s_i is the amount of heat at point i, and $R_i =$ input heat to the reactor.

The overall energy balance equation is calculated by equation 4.

$$\sum_{i=1}^{NC} \frac{F_i(z) \times C_{pmi}(z)}{M_{Wi}(z)} \times \frac{dT(z)}{dZ} = \frac{\dot{Q}}{L} + \frac{\pi \times D_i^2}{4} \times \sum_{j=1}^{NR} r_j(z) \times \Delta H_{rj}(z) \tag{4}$$

Hence, the energy balance equation which is used in Fluent software is as equation 5;

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_i}(K_{eff}\frac{\partial T}{\partial x_i} - \sum_j h_j J_j + u_j(\tau_{ij})_{eff}) + S_h \tag{5}$$

Where T is the Temperature, u_i is the input potential energy, u_j is the output potential energy, τ_{ij} is the applied torque in both directions, J_j is the output diffusion term, s_i is the input thermal of chemical reactions, S_h is the output thermal of chemical reactions, K_{eff} is the effective conductivity, and E is the total energy.

2.2. Geometry of the Simulated Reactor and Mesh Property

The geometry properties of simulated reactor are statistically demonstrated in table 3 and the schematic of one set of coil in the simulated furnace with more detail resolution is depicted in figure 5.

Table3. *Geometry of the Simulated Reactor*

Coil length	95 meter
Length of each branch	13.5 meter
Coil diameter	0.134 meter
Radius of the bend	0.178 meter

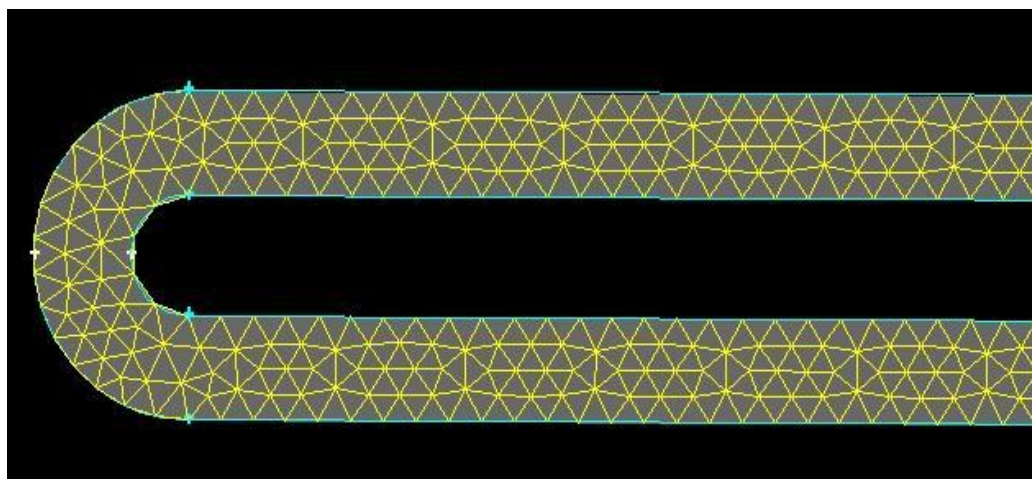| Length of the bend	0.500 meter
Number of bend	9
Thickness of the wall	0.800 meter

Figure5. *One Set of Coil in the Simulated Furnace with More Detail Resolution*

Furthermore, the properties of productive mesh are described in table 4.

Table4. *Properties of Productive Mesh*

Mesh interval size	0.03
Total elements	165469

Thermo- Physical Properties of Coil are clearly explained in table 5;

Table5. *Thermo- Physical Properties of Coil*

(K) Temperature	W/m.K)) Conductivity Factor
373	15.9
573	19
753	21.2
973	25.7
kg/m^3)) Density	8470
j/kg.k)) Thermal Capacity	444

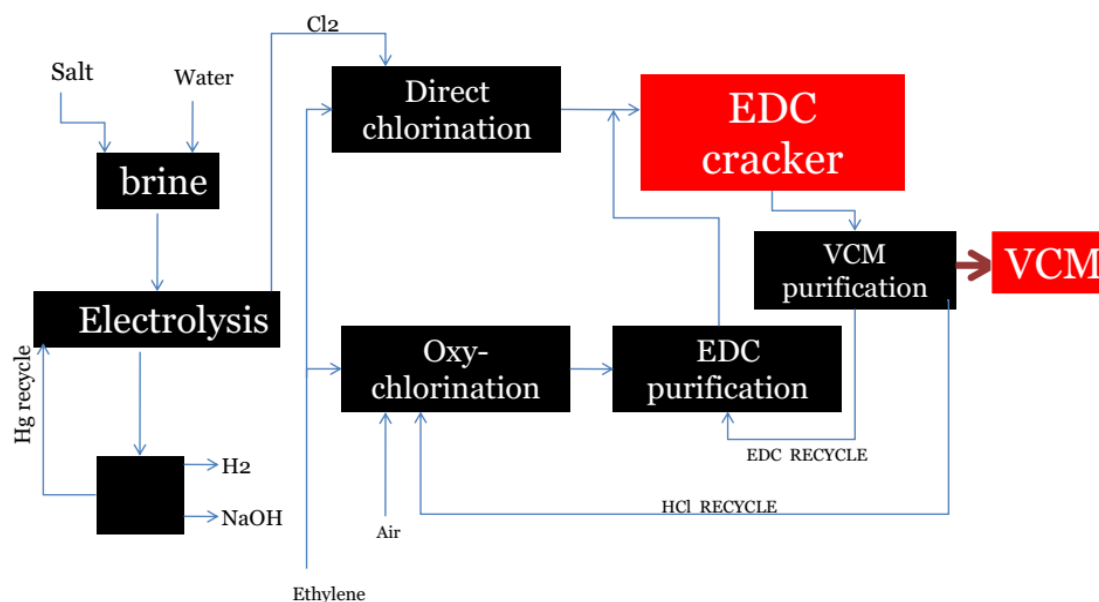The overall schematic of EDC thermal cracking unit in the simulated furnace is plotted in figure 6.

Figure6. *Schematic of EDC Thermal Cracking Unit in The Simulated Furnace*

2.3. FLUENT Software

FLUENT Software is one the engineering software for simulating and modelling the operational processes and procedures in petrochemical industries to obtain the appropriate estimation of chemical reactions and analyse the considerable influence of each parameter. The software creates simulated computer models of structures, electronics, or machine components to simulate strength, toughness, elasticity, temperature distribution, electromagnetism, fluid flow, and other attributes.

2.4. Inlet and Output Flow

The fluid conditions of input and output flow is described in table 6 and 7;

Table6. *Input fluid conditions*

Feed mass flow rate	kg/s 6.086
mass percentage of Input EDC	0.9707
mass percentage of Input VCM	0.0184
mass percentage of HCL input	0.0109

Table7. *Applied boundary conditions for output flow in the software.*

location	Type of boundary condition
Walls	Heat flux
Input gas	Input mass rate
Output flow rate	Output pressure

2.5. Parameters of The Simulated Model

The parameters which are used in this research are described statistically in table 8;

Table8. *Parameters of the Simulated Model*

Parameter	Standard k-ϵ Model
C_D	0.09
C_1	1.44
C_2	1.92
σ_k	1
σ_ε	1.3

3. RESULTS AND DISCUSSION

3.1. Selection of Appropriate Mesh

To do this, in the simulation processes, five types of mesh are being taken into consideration and they are compared together. As can be seen in table 9, EDC conversion factor for the sets of mesh with the numbers of 172351 and 165649 are the most according to the results of simulation and it would be preferred for the experimental evaluation.

Table9. *Selection of Appropriate Mesh*

Number of Mesh	EDC Conversion Factor
98452	47.05
125893	49.1
148216	50.8
165649	52.69
172351	52.69
Experimental Amount	48.4

3.2. Fluid Temperature in the Coil Length

Fluid temperature is one of the most considerable parameter which seriously affect the total procedures in the furnace. According to figure 7, the temperature alteration for the mixture at initial steps is drastically high, hence the temperature raised relatively 40 k. This temperature enhancement will continue up to about 45 meters of reactor length. Since then, the temperature is increased at the final length of the reactor; in respect of the way, the temperature rises so slowly at 105 meters in the final lengths. The reason for this is that, at the beginning of the reactor length, failure reactions have not yet begun, and much of the heat flux applied to the reactor is simply to increase the temperature of

the gas mixture. In fact, the feed is preheated before entering the reactor. Although, it is necessary to prevent the initiation of defective reactions in the pre-heating zone, it is usually used in the first few meters of the applied heat exchanger to merge the mixture to the reaction temperature and basically there is no reaction in this area.
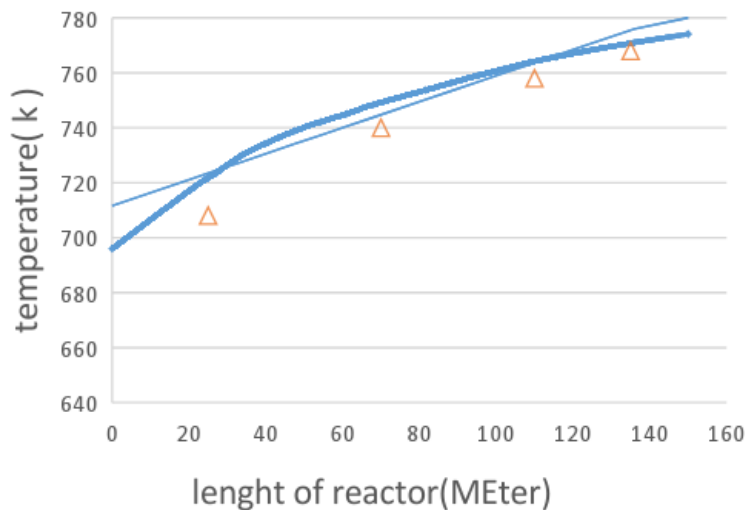

Figure7. Effect of Temperature on the Procedure

3.3. EDC Mass Fraction Alteration

Due to temperature soaring in the reactor, the conversion factor will be increased subsequently. Thereby, at the end length of the reactor, the conversion factor reaches the peak (it is approximately 53%). In addition, EDC mass fraction in the inlet and at the outlet are 0.97 and 0.46 respectively. The plot of EDC mass fraction in the reactor length of is graphically shown in figure 8.
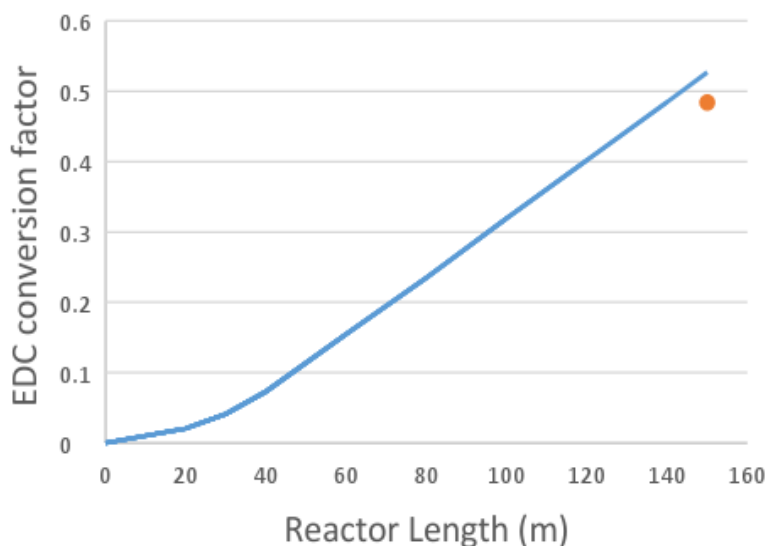

Figure8. *EDC Mass Fraction Alteration*

3.4. VCM Mass Fraction Alteration

At the beginning stages of the process, the applied heat in which is received from the furnace is used to increase the temperature of processing fluid is very low. Next, due to the progress of the procedure this amount will be increased significantly. Therefore, VCM mass fraction at the inlet and outlet are measured 0.018 and 0.23 respectively. It should be noted that a small amount of VCM at the inlet is regarding the result of feedback. This phenomenon is clearly depicted in figure 9.
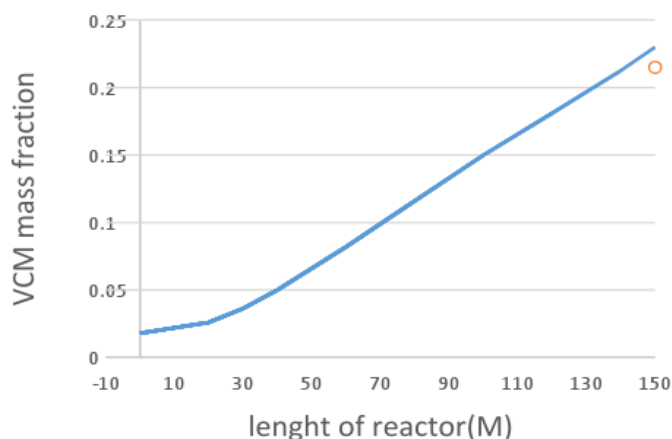
Figure9. *VCM Mass Fraction Alteration*

3.5. Pressure Profile Alteration

At the beginning of the process, the pressure drop in coils is very low which is be negligible. Since then, it seems a gradual increase with the reaction progress in the reactor and at the end of coils pressure drop will be increased drastically. Pressure profile alteration is shown in figure 10.
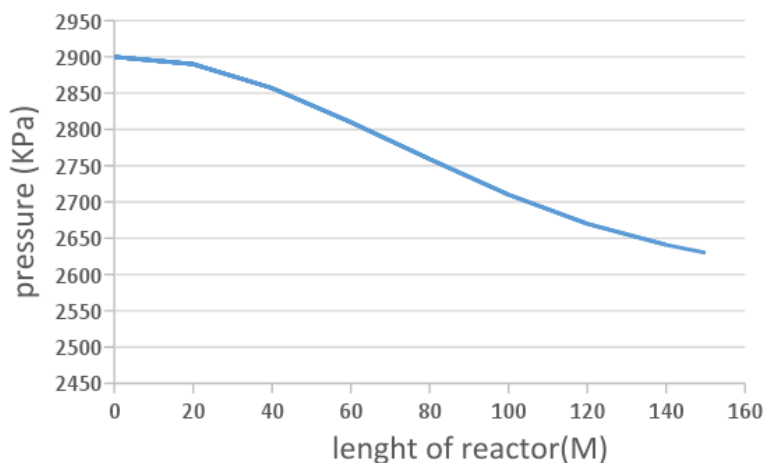

Figure10. *Pressure Profile Alteration*

Moreover, the EDC conversion factor is calculated for different equilibrium equations are explained in table 10.

Table10. *EDC conversion factor for different equilibrium equations*

Gas Equilibrium Equations	EDC Conversion Factor
Ideal Gas	52.69
Peng Robinson	51.42
Redlich Kwong	50.78
Soave-Redlich Kwong	50.45
Aungier-Redlich Kwong	49.75
Industrial Experimental Data	48.4

4. CONCLUSION

In this research FLUENT software is used for EDC thermal cracking procedures simulation in 2-D model. Due to the effective parameters which are fundamentally impact the cracking processes in the furnace, EDC conversion factor will be increased by increasing the temperature profile in the furnace. Moreover, Non-ideal assumption effects of processing fluids were also taken into consideration by administering the real gas. Therefore, the obtained conversion factor is seems more closer to industrial purposes.

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