# KINETIC MODELING AND DESIGN OF AUTOCLAVE REACTOR FOR DEHYDROGENATION OF PROPANE TO PROPYLENE

## ABSTRACT

This research was carried out following the high demand of propylene as a precursor to polypropylene plastic and packaging materials as a trending problem to the packaging industries. Its main focus is on kinetic modeling and Design of an Autoclave reactor for the dehydrogenation of propane to propylene. its aim is to develop an appropriate kinetic model for propane dehydrogenation (PDH) Over an industrial pt - Sn/c - A1203 Catalyst in the presence of small amounts of Oxygenated Compounds Experimental data were obtained from a previous where catalytic PDH was carried out in a laboratory scale reactor at atmosphere pressure in the temperature range of 575-620°C in the presence of small amounts of water or Methanol. The kinetics of the main dehydrogenation reaction was described and the effects of water and methanol on coke deposit ion and catalyst sintering were considered in a catalyst deactivation model to explain the observed optimum level in the amount of added oxygenated compounds. Analysis of the designed autoclave reactor was assessed equivalently to the performance evaluation of the autoclave reactors for dehydrogenation of propane at Variant process temperature using MATLAB algorithm and programming integrations. The volume of the propylene formed from the system increases with increase in the reactors process temperature. Same as the depletion rate those such that there is a Ore accelerative proportional in Crease in the propylene volume from 34.8205 $m^3$ 24.3744$m^3$, 31.3385 $m^3$ 51.4815 $m^3$, 66.1906 $m^3$ within 60% to 90% fractional Conversion of the system, assessed on the basis of Variant temperatures 250°C, 350°C and 450°C respectively.

**Keywords:** Propane Dehydrogenation, Propylene, Autoclave Reactor, Kinetic Modeling

## 1. Introduction

Propylene Commonly referred to a propene; with a molecular formula of C3H6, is an organic compound belonging to the alkene family which are the olefins, with general molecular formula of CnH2. It is regarded as a third member of the organic homologous series, and an active reactive gas (Nauman et al, 2004). Stated the propene is not usually a naturally occurring constitute of Crude oil as earlier posited, but has multiple source of regeneration from Crude oil and natural gas. Propylene is a key intermediate in the chemical industry, used in the production of polypropylene and as a by-product of steam cracking. Traditionally produced as a by-product of cracking, the growing demand necessitated alternative production routes. Propane dehydrogenation (PDH) has emerged as an attractive method for producing propylene.

The reaction is highly endothermic and reversible.

Given the Equation: $C_3H_8 = C_3H_6 + H_2$.

Due to equilibrium limitations and catalyst deactivation, efficient reactor design and kinetic understanding are critical. PDH has been considered as a high selectivity route for the production of propylene. Pt-Sn Catalysts exhibit more advantages than other catalysts due to high selectivity and stability in the dehydrogenation of paraffins to olefins.

## 2. Materials and Methods

The research adopted a mathematical approach derivatives and Simulative evaluation which subjected it to a non-experimental materials, which are.

i. Auto CAD

ii. MATLAB Computer program.

iii. Computer set

iv. Hand books and journals in chemical Engineering.

### 2.1 Methods

Experimental setup

### 2.1.1 Process decryption of propane Dehydrogenation to propylene

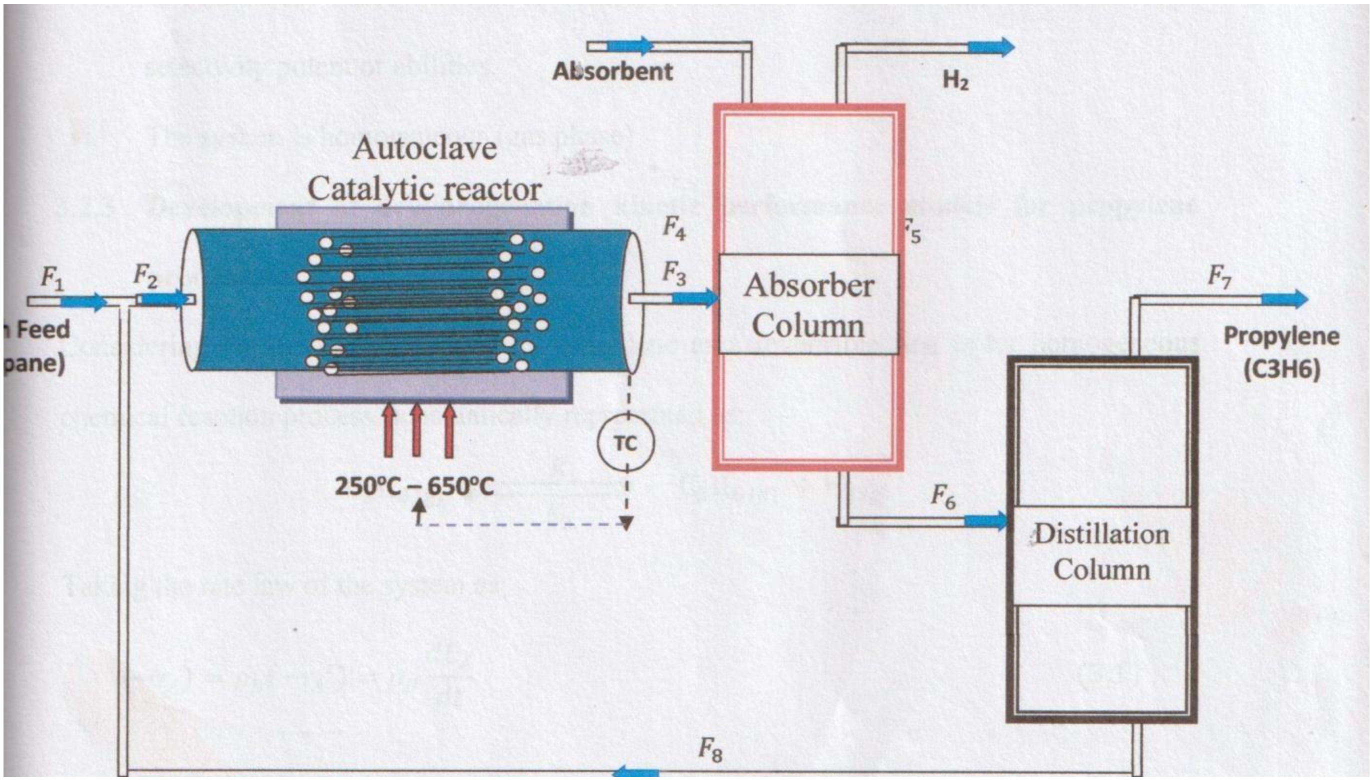

Fig. 1: Shows the process description of dehydrogenation unit for propylene production

A. Laboratory-scale high-pressure batch autoclave reactors fabricated from stainless steel (SS316) with a total volume of 1-2 L. And the reader equipped with.

I. An internal mechanical stirrer (0-1000 rpm) for uniform making:

II. Electric heating mantle with PID temperature control (+1K accuracy)

III. Pressure gauge and safety relief valve.

IV. Thermocouple inserted into the reaction mixture

V. Gas inlet/outlet valves for charging and sampling

### 2.2 Reaction Procedure

Prior to each experiment, the reactor was purged with nitrogen to eliminate oxygen and prevent unwanted side reactions. A known mass of catalyst (typically 5-20 g) was loaded into the reactor.

The system was then charged with propane to the desired initial pressure (1-10 bar). The reactor temperature was increased to the operating range of 500-650 °C, which is typical for PDH reactions.

Once the set temperature was reached, stirring was initiated to ensure homogeneous mixing. Reaction time varied between 30 and 180 minutes depending on the experimental conditions.

Gas samples were periodically withdrawn and analyzed to determine propane conversion and product distribution.

### 2.3 Analytical methods

Product analysis were carried out using gas chromatography (GC) equipped with the following:

1. Flame Ionization Detector (FID) for hydrocarbon

II Thermal Conductivity Detector (TCD) for hydrogen

Separation of the components was achieved using a capillary column suitable for lighter hydrocarbons

The following performance metrics were calculated: propane conversion

(Xp)= $\frac{F_{c3}\ H_8^{m}\ F_{C3}\ H_8}{F_{c3}\ II_8^{in}}$ and

Propylene selectivity (Sp):
Sp = $FC_3H_6$
$FC_3H_8$

and

yielded propylene (Yp)
Yp = Xp x Sp

A Langmuis- Hmshelwood-Hougen-Wasson (LHAW) Kinetic model was adopted to account for surface adsorption and reaction mechanisms. The general rate expression used was.

r= $KP_3H_8$

$(K_1KC_3H_8P_3 \| K_2P_{02})^2$

where:

r = reaction rate (mol/Kg.s)

K = rate constant (temperature-dependent)

K = adsorption equilibrium constant

Pi = Partial pressures of species

The temperature dependence of the rate constant followed the Arrhenius equation

$$K = \frac{A\ \exp(-Ea)}{R^T}$$

Nonlinear regression techniques (e.g. least squares fitting using MATLAB or python) were employed to estimate kinetic parameters from experiment data.

## 2.4 Reactor Design modeling

The autoclave reactor was modeled as a batch reactor system with the following mole balance:

$$\frac{dNA}{dt} = rV$$

where NA = number of moles of propane

V = reactor Volume.

Energy balance method was also incorporated to account for the endothermic nature of the dehydrogenation reaction:

$$Q = \frac{mCp\ dT + \Delta Hr \times rV}{dt}$$

Statistical indicators such as $R^2$, RMSE, and residual and analysis were used to evaluate the model accuracy.

## 3. Results and Discussion

This chapter delves into the mathematical models of the autoclave reactor design for propylene formation from propane dehydrogenation reaction System.

The developed kinetic model for propane dehydrogenation (PDH) in an autoclave reactor was validated against experimental and literature data.

The reaction network primarily follows the endothermic dehydrogenation pathway. With its results achieved using the MATLAB, it consists of the results of the fractional conversion effects on autoclave reactor depletion performance in propane dehydrogenation system. Result obtained from MATLAB Simulation System, and the relationship between conversion and autoclave reactors volume performance.

**The below Table shows the mathematical data obtained from MATLAB Simulation of the System**.

| **XA** | **$C_A$-250 ($mol/m^2$)** | **$C_A$-350 ($mol/m^2$)** | **$C_A$-450 ($mol/m^2$)** | **$C_D$- 250 ($mol/m^2$)** | **$C_D$- 350 ($mol/m^2$)** | **$C_D$- 450 ($mol/m^2$)** | **$V_R$-250 ($m^3$)** | **$V_R$-350 ($m^3$)** | **$V_R$-450 ($m^3$)** |
|---|---|---|---|---|---|---|---|---|---|
| 0.1000 | 54.7292 | 55.3836 | 54.9456 | 2.2384 | 1.5840 | 2.0220 | 4.7160 | 3.3012 | 4.2444 |
| 0.2000 | 52.5434 | 53.7989 | 52.9537 | 4.4242 | 3.1687 | 4.0139 | 9.7172 | 6.8020 | 8.7455 |
| 0.3000 | 50.3826 | 52.1920 | 50.9732 | 6.5850 | 4.7756 | 5.9944 | 15.0801 | 10.5560 | 13.5721 |
| 0.4000 | 48.2245 | 50.5525 | 48.9791 | 8.7431 | 6.4131 | 7.9885 | 20.9165 | 14.6415 | 18.8248 |
| 0.5000 | 460.344 | 48.8489 | 46.9371 | 10.9332 | 8.1187 | 10.0305 | 27.3998 | 19.1798 | 24.6598 |
| 0.6000 | 43.7606 | 47.0340 | 44.7999 | 13.2070 | 9.9336 | 12.1677 | 34.8205 | 24.3744 | 31.3385 |
| 0.7000 | 41.3138 | 45.0266 | 42.4814 | 15.6538 | 11.9410 | 14.4862 | 43.7234 | 30.6064 | 39.3510 |
| 0.8000 | 38.5046 | 42.6500 | 39.7930 | 18.4630 | 14.3176 | 17.1746 | 55.3310 | 38.7317 | 49.7979 |
| 0.9000 | 34.7915 | 39.3940 | 36.2021 | 22.1761 | 17.5736 | 20.7666 | 72.5451 | 51.4815 | 66.1906 |

Table showing assessment of Reactor Depletion Rate on fractional conversion basis

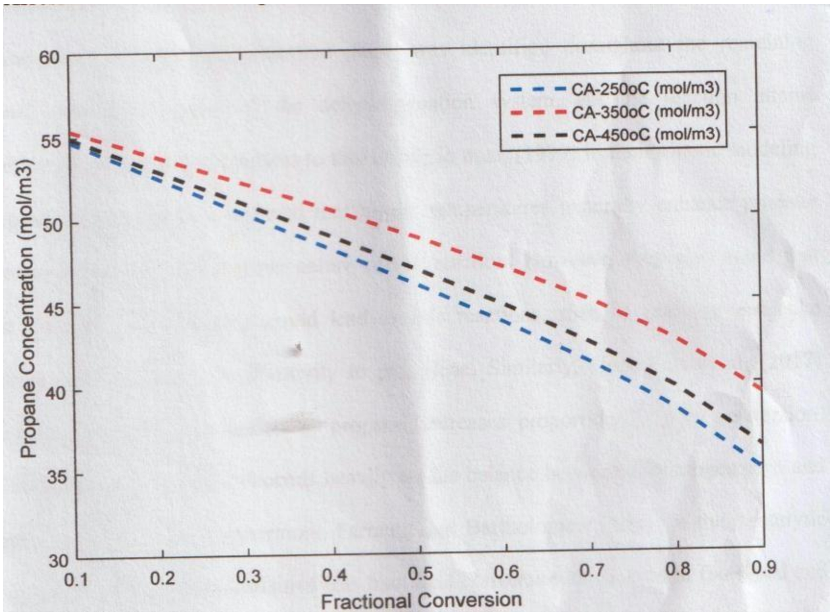

Fig. 2 showing Fractional Conversion

Figure 2 Fractional Conversion effects on autoclave reactor depletion performance in a propane dehydrogenation system. and formation of propylene. It was identified that the depletion of the propane concentration increases with increase in temperature, especially at temperature as assessed using 250°C, 300°C and 450°C autoclave reactor temperature.

The results displayed in Figure 2.2 as obtained from appendix 1 depicts the relationship between the fractional conversion of propane in an autoclave reactor and the reactant concentration gradient at different process temperature basis. The result shows that the concentration of the propane depletes proportionally with increase in the process conversion and formation of propylene. It was also identified that the depletion of the propane concentration increases with increase in temperature, especially at a temperature as assessed using 250°C, 300°C and 450°C autoclave reactor temperature, which promotes respectively the depletion of 56.9676 mol/m$^3$ propane to 34.7915 mol/m$^3$, 39.3940 mol/m$^3$ and 36.2021 mol/m$^3$, yielding propylene of 22.1761 mol/m$^3$, 17.5736 mol/m$^3$ and 20.7655 mol/m$^3$ concentration.

During the conversion process, as resulted from the study, the system experiences a steady depletion rate of the 56.9676 mol/m$^3$ propane fed into the autoclave reactor from 10% to 76.5% fraction conversion of the propylene formation system, then a slow and more depleting concentration phase was identified throughout the remaining fractional conversion stages of the dehydrogenation system, till the reaction attains completion.

This finding corroborates to that of Marin et al. (1999) in their kinetic modeling of propane dehydrogenation reported that higher temperatures generally enhance propane conversion due to the endothermic nature of the reaction. However, they also noted that excessive temperature increases could lead to side reactions, such as cracking and coke deposition, which reduce the selectivity to propylene.

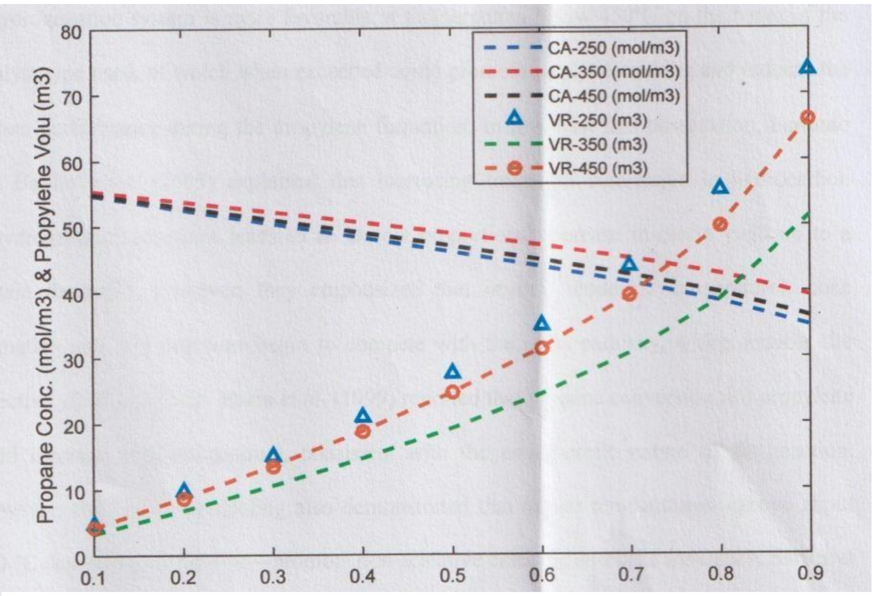

Fig 3. Predicts the Fractional Conversion effects on volume of propylene formed in the propane dehydrogenation system

Figure 3 obtained from presents the relationship between change in fractional conversional effects on the volume of propylene formed in the system on the bases of propane depletion due to dehydrogenation at variant process temperatures of an autoclave reactor. The results depict that increase in fractional conversion of the system promotes the propylene volume formation which is as a result of the continual depletion of the propylene concentration over a defined process space time. The volume of the propylene formed from the system increases with increase in the reactor's process temperature, same as the depletion rate those, such that the there is a ore accelerative proportional increase in the propylene volume from 34.8205 m³ 24.3744 m³, 31.3385 m³ to 73.5451 m³, 51.4815 m³, 66.1906 m³ within 60% to 90% fractional conversion of the system, assessed on the basis of variant temperatures 250°C, 350°C and 450°C respectively, resulted from the depletion of 56.9676 mol/m³ propane feed within same system conversion range. The result also show that the dehydrogenation system is more favorable at temperatures below 450°C on the bases of the catalyst type used, of which when exceeded could promote catalytic cocking and reduces the system performance during the propylene formation. In line with this observation, Farrauto and Bartholomew (2005) explained that increasing fractional conversion in hydrocarbon dehydrogenation reactions leads to an almost proportional increase in olefin yield up to a certain threshold. However, they emphasized that beyond moderate temperatures, coke formation and side reactions begin to compete with the main pathway, which reduces the effective yield.

## 4. Conclusion

The Kinetic modeling reactor design analysis showed that the auto clave reactor configuration can achieve high propane conversion and propylene selectivity under optimized operating conditions, high temperature, moderate temperature and controlled residence time. Heat transfer limitations and mass diffusion effects were identified as critical parameters influencing reactor performance emphasizing the need for efficient thermal management and mixing within the system. The model also highlighted the sensitivity of propylene yield to operating variables such as temperature, feed composition, and catalyst loading.

Simulation results indicated that optimal performance is achieved within a narrow operating window, where equilibrium limitations are balanced with reaction kinetics to maximize propylene production while minimizing undesired by-products. The integration of kinetic modeling with reactor design provides a valuable tool for scaling up the process and guiding industrial application in the petrochemical industries.

This research work contributes to the advancement of propane dehydrogenation technology by offering a robust modeling approach and practical design insights for autoclave reactors.

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