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Aspen HYSYS Guided Modelling in the Transesterification of Palm Oils for Customization as Drilling Fluids Additive

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Abstract

This paper discusses the advancements in earlier studies on transesterification of palm oils; here we are presenting advanced Aspen HYSYS modelling of different complexities of hierarchical layers of simulation aimed at customizing esters derived from palm oils for different application. Published studies in transesterification show products from various vegetable oils for different applications including biodiesel production and drilling fluids formulation. In general, vegetable Oils consist of triglycerides (TG) 90 - 98 % by weight, small diglycerides (DG) and monoglycerides (MG), while palm oil contains TG 95.7%, DG 3.7%, and MG 0.6%. In the catalysis of transesterification of vegetable oils with alcohol, TG is converted stepwise to DG, MG and finally glycerol (GL). These reactions were modelled in varied layers of complexities in Aspen HYSYS: flowsheeting, steady state, sensitivity analysis, optimization and transient conditions in a CSTR at varied reaction conditions and time to produce varied esters properties.

Results from the models demonstrate the reliability of the various layers of the complexities of the simulation; show properties of the esters at various process conditions and therefore reveals prospects for customizing these esters derived from the transesterification of palm oils for various applications. Overall, the results show that this approach can guide further laboratory and modelling research towards customizing palm oil as drilling fluid additive.

Keywords: Transesterification; Complexities; Customization; Esters; Modeling; Reactions.

1. Introduction

This study aims at advancing the objective of customizing palm oils as drilling fluids additive. The approach requires that with transesterification studies, a guided stage-wise process will enable the catalytic and other modelling method to be used to determine appropriate physical and thermodynamic properties of the ester to meet the requirements as additive. The transesterification done here uses advanced Aspen HYSYS modelling [1] to determine these parameters based on published available data on palm oils, drilling fluids and applicable additives. The outcome of this modelling will guide the systematic laboratory customization of palm oils as drilling fluids additives.

This study is also designed to contribute to the on-going research on palm oil esters for different applications, including the use for drilling fluid [2-5]. Kinetics used in these studies has been by transesterification with alcohol with assumptions made to simplify the sets of differential equations to eliminate the effect of acidity on the reaction. We have made similar assumptions in the Aspen HYSYS model presented here.

2. The Transesterification in Customizing Palm Oil for Additive in Drilling Fluids Formulation

Transesterification is a chemical reaction that can be used to customize palm oil **(Table 1)** to be used as an additive for drilling fluids formulation. During transesterification reaction, palm oil is reacted with an alcohol (e.g., methanol or ethanol) in the presence of a catalyst (e.g., sodium methoxide) to produce fatty acid methyl esters (FAMEs) or fatty acid ethyl esters (FAEEs). The transesterification reaction can enhance the properties of palm oil to meet drilling formulation requirement by: reducing the viscosity of palm oil; improved lubricity of FAMEs or FAEEs compared to palm oil; increased thermal stability of the palm oil making it more resistant to degradation at high temperatures; enhanced emulsification of FAMEs or FAEEs over palm oil, allowing it to form stable emulsions with water.

The transesterification reaction can be customized to produce FAMEs or FAEEs with specific properties by: choosing the right alcohol - methanol or ethanol can be used to produce FAMEs or FAEEs with different properties; selecting the catalyst - different catalysts can be used to control the reaction rate and selectivity; controlling reaction conditions - temperature, pressure, and reaction time can be adjusted to optimize the reaction.

The resulting FAMEs or FAEEs can be blended with other additives or base oils to formulate a drilling fluid with the desired properties.

Table-1. Typical composition of palm oil

S/N	Property	Quality
i	Saturated Fat	50% of palm oil is made up of saturated fats, which are considerably less than palm kernel oil
ii	Monounsaturated Fat	40% of palm oil is made up of monounsaturated fats
iii	Polyunsaturated Fat	10% of palm oil is made up of polyunsaturated fats
iv	Triglycerides	Palm oil contains triglycerides, which are separated from other components through refining
v	Vitamin A	Palm oil is a source of Vitamin A
vi	Vitamin E	Palm oil is a source of Vitamin E
vii	Beta-Carotene	Palm oil contains beta-carotene, which gives it a reddish color
viii	Free Fatty Acids	Palm oil contains free fatty acids, which are removed during the deodorizing process

3. Reactions and Kinetics for transesterication of Palm Oils

Transesterification of palm oil involves the conversion of triglycerides into fatty acid methyl esters (FAMEs) or biodiesel. The reactions and kinetics are as follows:

Triglyceride (TG) + Methanol (MeOH) ⇌ Diglyceride (DG) + Fatty Acid Methyl Ester (FAME) ***1***

DG + MeOH ⇌ Monoglyceride (MG) + FAME ***2***

MG + MeOH ⇌ Glycerol (Gly) + FAME ***3***

Kinetics:

(i) The transesterification reaction is typically catalyzed by an acid or base.

(ii) The reaction rate is influenced by factors such as temperature, pressure, reactant concentrations, and catalyst type.

(iii) The kinetics can be described by the following rate equation:

$$r = k\,[TG]\,[MeOH] / (1 + [MeOH] / K) \qquad \textbf{4}$$

where r is the reaction rate, k is the rate constant, [TG] is the triglyceride concentration, [MeOH] is the methanol concentration, and K is the equilibrium constant.

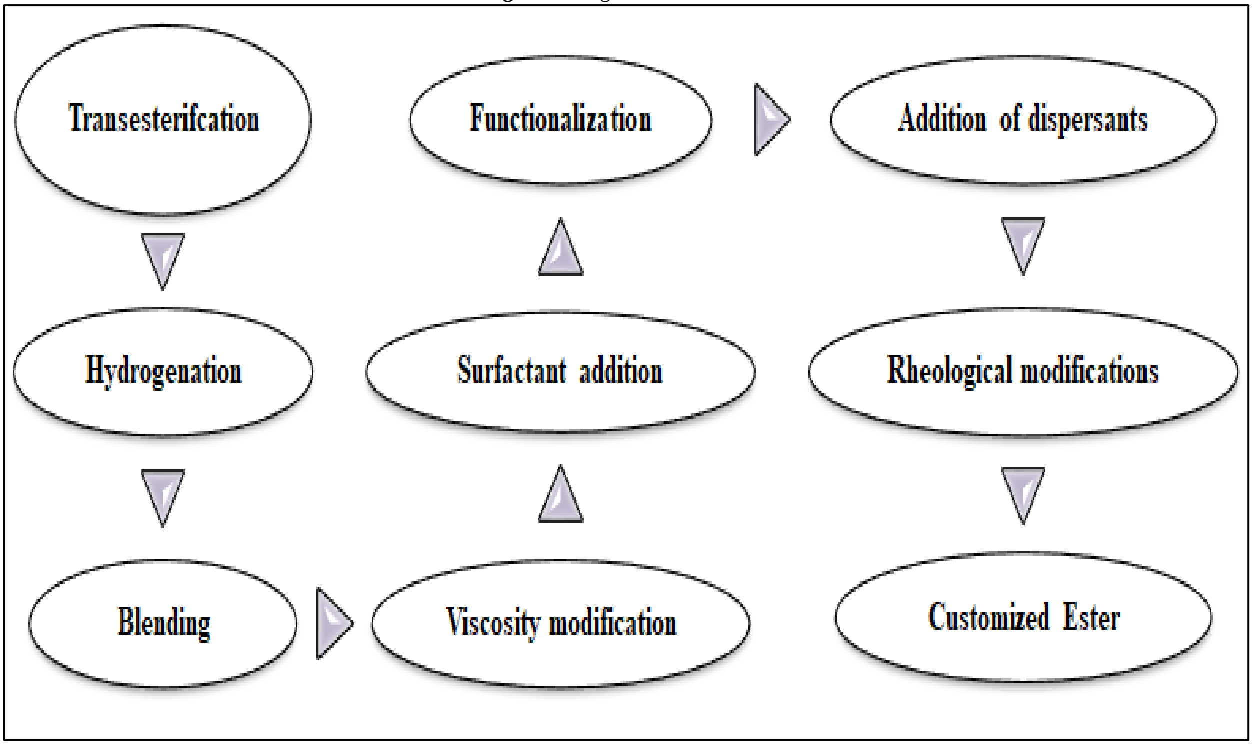
The activation energy for the transesterification reaction is typically around 50-70 kJ/mol. The reaction is usually conducted at temperatures between 50-200°C and pressures between 1-10 bar.

4. Customization of Palm Oils as Additive Drilling Fluids Formulation

Palm oils can be customized to be used as an additive for making drilling fluids by the following steps as represented in Figure 1.

- **Transesterification**: converts palm oil into fatty acid esters to improve its lubricity and thermal stability.
- **Hydrogenation**: reduces the unsaturation in palm oil to increase its stability and viscosity index.
- **Blending**: mixes palm oil with other additives or base oils to achieve the desired properties.
- **Functionalization**: chemically modifies palm oil to introduce functional groups that enhance its performance in drilling fluids.
- **Surfactant addition**: adding surfactants to palm oil to improves its emulsification properties.
- **Viscosity modification**: adjusts the viscosity of palm oil to meet the requirements of drilling fluids.
- **Addition of dispersants**: adding dispersants to palm oil to improves its stability and prevent settling.
- **Rheology modification**: modifies the rheological properties of palm oil to improve its flow behavior.
- **Customized Ester**: formulated and customized ester

Figure-1. Stages in Transesterification



These customizations can enhance the properties of palm oil, making it suitable for use as an additive in drilling fluids, such as: adjusted viscosity to achieve the desired flow behavior and pressure drop in the drilling fluid; enhanced lubricity to reduce friction between the drill pipe and the wellbore, improving drilling efficiency; improve emulsification properties to stabilize the drilling fluid's water-oil ratio and prevent phase separation; increase thermal stability is increased to withstand the high temperatures encountered during drilling operations; improve dispersibility to ensure uniform distribution in the drilling fluid and prevent settling; modify rheological properties to achieve the desired flow behavior, such as pseudoplastic or dilatant behavior. Other expected improvements of the palm oil through customization include; enhance stability is enhanced to resist degradation and maintain its properties over time; adjusting other properties to optimize filter cake formation and improve wellbore stability; improving HTHP performance to maintain its properties under extreme conditions; and evaluate potential palm oil's environmental impact to minimize its footprint and ensure biodegradability.

By targeting these properties, customized palm oil additives can enhance the performance and efficiency of drilling fluids, leading to improved drilling operations and reduced environmental impact. Transesterification plays a crucial role in customizing palm oil for use as an additive in drilling fluids by

- **Converting triglycerides**: transesterification converts palm oil's triglycerides into fatty acid methyl esters (FAMEs), which improves its lubricity and thermal stability.
- **Improving solubility**: transesterification enhances the solubility of palm oil in drilling fluids, ensuring uniform distribution and preventing settling.
- **Enhancing emulsification**: transesterification improves palm oil's emulsification properties, stabilizing the water-oil ratio and preventing phase separation.
- **Modifying viscosity**: transesterification allows for the adjustment of palm oil's viscosity to achieve the desired flow behavior and pressure drop in the drilling fluid.
- **Increasing thermal stability**: transesterification increases palm oil's thermal stability, enabling it to withstand high temperatures during drilling operations.
- **Improving dispersibility**: transesterification enhances palm oil's dispersibility, ensuring uniform distribution in the drilling fluid and preventing settling.
- **Optimizing rheology**: transesterification allows for the modification of palm oil's rheological properties to achieve the desired flow behavior.

By converting palm oil into FAMEs through transesterification, the resulting palm oil additive will have improved properties, in the range listed in **Tabe 2** below, making it suitable for use in drilling fluids with the range defined in **Table 3** below.

Table-2. Properties targeted in the customization of palm oils

	Property	Targeted	Remarks
(a)	Viscosity	10-100	10-100mm²/s (millistokes) at 40°C
(b)	Lubricity	50-100	50-100% improvement in lubricity compared to base oil
(c)	Emulsification		Stable emulsion with 20-50% water content
(d)	Thermal stability	200-300	200-300°C (392-572°F) without significant degradation
(e)	Dispersibility	90-100	90-100% dispersible in drilling fluid
(f)	Rheology		Pseudoplastic or dilatant behavior with a viscosity index of 100-200
(g)	Stability		No significant degradation or settling over 24 hours at 150°C (302°F)
(h)	Filter cake formation	10-50	10-50% reduction in filter cake thickness
(i)	HTHP performance		Stable performance at 200-300°C (392-572°F) and 100-200 bar (1450-2900 psi)
(j)	Environmental impact		Biodegradable and non-toxic

Table-3. Typical specification for drilling fluids

	Property	Targeted	Units
(a)	Density	1.02-1.49	g/cm3
(b)	Viscosity	10-100	cP (centipoise)
(c)	pH	8-12	
(d)	Alkalinity	0-10	meq/L (milliequivalents per liter)
(e)	Filtrate volume	5-15	mL
(f)	Filter cake thickness	1-5	Mm
(g)	Lubricity	50-100	% improvement over base oil
(h)	Emulsification	20-50	stable emulsion with 20-50% water content
(i)	Thermal stability	200-300	°C
(j)	Dispersibility	90-100	% dispersible in drilling fluid
(k)	Rheology	100-200	pseudoplastic or dilatant behavior with a viscosity index of 100-200
(l)	Stability	150	no significant degradation or settling over 24 hours at 150°C (302°F)
(m)	HTHP performance	200-300	stable performance at 200-300°C (392-572°F) and 100-200 bar (1450-2900 psi)
(n)	Environmental impact		biodegradable and non-toxic

5. Drilling Fluids type for Palm Oil Customization as Additive

It's important to note that drilling fluids are typically classified into different types, such as: Water-based drilling fluids (WBDF); Oil-based drilling fluids (OBDF); Synthetic-based drilling fluids (SBDF); Foam drilling fluids (FDF).

Customized palm oil will likely be used as an additive in: Water-Based Drilling Fluids (WBDF) to enhance lubricity, improve emulsification, increase thermal stability and reduce friction and wear on drilling equipment; or Synthetic-Based Drilling Fluids (SBDF) to improve rheological properties, enhance thermal stability, increase dispersibility and reduce environmental impact. **Table 4** should be a basis and a guide for evaluation of the quality of the selected palm oil.

Table-4. Typical composition with numbers and characteristics of palm that qualifies it to be used as drilling fluids additive

A. Composition			**B. Characteristic**		
	Component	**Typical (%)**		**Property**	**Typical**
(i)	Palmitic acid	40-50	*(i)*	Viscosity, mm²/s	10-50
(ii)	Oleic acid	30-40	*(ii)*	Density, g/cm³	0.9-1.0
(iii)	Linoleic acid	5-10	*(iii)*	Flash point, °C	200-250
(iv)	Stearic acid	2-5	*(iv)*	Pour point, °C	10 to 0
(v)	Other fatty acids	1-2	*(v)*	Lubricity, %	50-100
			(vi)	Emulsification, %	20-50
			(vii)	Thermal stability, °C	200-300
			(viii)	Dispersibility, %	90-100

6. Hierarchies and Complexities in Process Analysis and Modelling

In general, the concept takes its hierarchy from Figure 2A illustrated as an ***onion*** below, a principle in process analysis: catalysis is modelled first with selected kinetics (Figure 3)[1]. Thereafter the separation and recycle systems are integrated; this continues to the outer section of the ***onion.***

In the Aspen HYSYS modelling the hierarchy incorporates the complexities as shown and illustrated as an ***onion*** in Figure 2B below: beginning from the heart of the model - the reactor and the kinetic model, the approach goes through the other layers, namely flowsheeting, steady state, case studies/sensitivity analysis to the dynamic/transient analysis. Each layer was subjected to intensive and robust analysis to proof the concepts and the reliability of the models.

Figure-2. Hierarchies in Process Analysis and Aspen HYSYS modelling

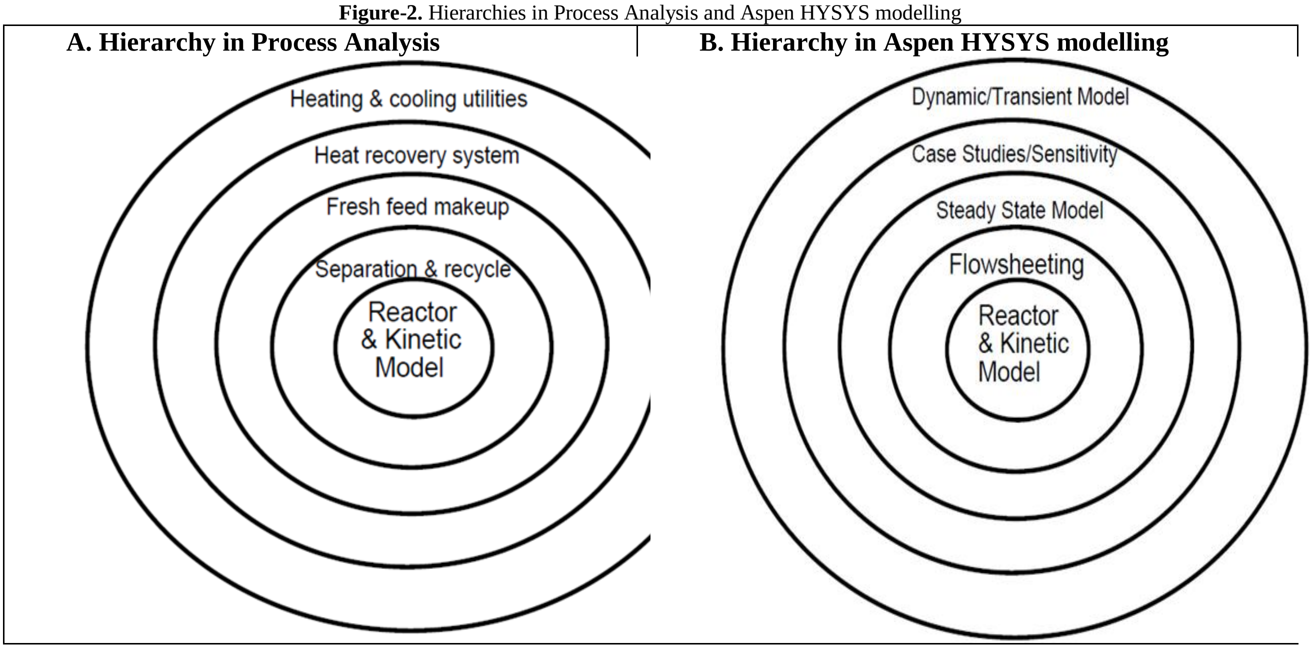
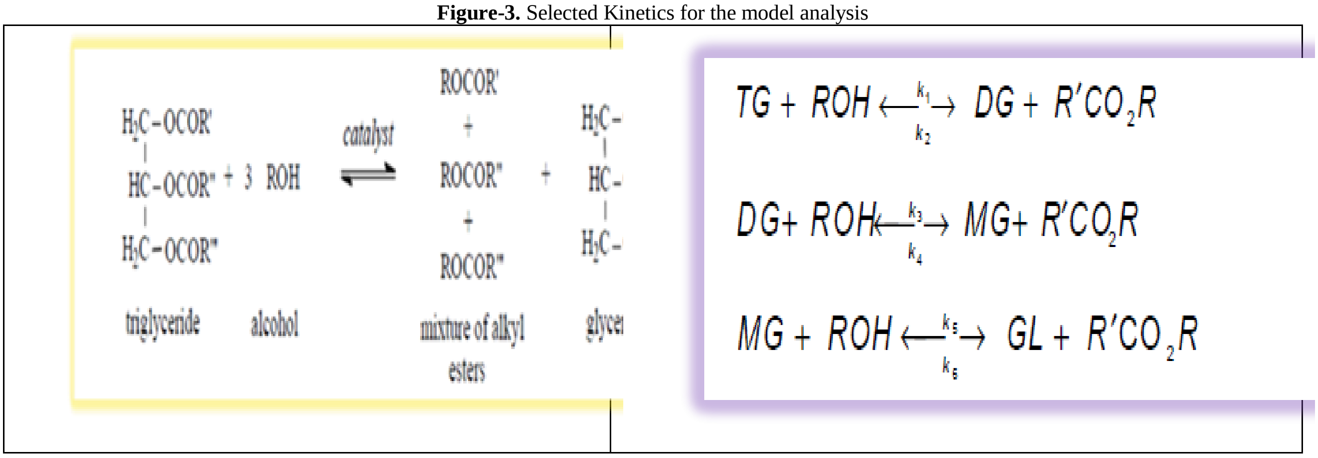


Figure-3. Selected Kinetics for the model analysis



7. Results and Applications

Figure 4 shows the overall flowsheet developed and modelled based on the concepts and complexities in Figure 2 above. The outcome of the simulations is contained here: for steady state model and sensitivity analysis (Table 5, Figure 5); and dynamic/transient analysis (Figure 6).

The reliability of the models at varied complexities across the layers in Figure 2B above, has been fully demonstrated; the results obtained show prospects for modifying the physical & thermodynamic properties of the palm oil ester, by applying appropriate reaction conditions to customize the ester to meet various end use applications.

8. Discussion

We have presented here some insights into the transesterification of palm oils: the concept of transesterification and its peculiar catalysis; and palm oil feedstock characteristics to match target products' characteristics and process conditions. As this paper targets to contribute to the on-going research on palm oil esters for different applications, including the use for drilling fluid[2-5], we have selected key information and data for both this and future study aimed at expanding this subject further. The concepts, data on the palm oil and drilling fluids, and results from the Aspen HYSYS modelling of the transesterification have shown how, given tested concepts with appropriate data, can guide a fruitful, reliable and versatile process engineering modelling as presented here. The nature and complexity of the model are such that various palm oils, including other vegetable oils can be studied in this model: the essential differences, like oil characteristics and the appropriate kinetics will be applied as required, and modelling intensified at varied process conditions to give desired products properties. It is important to note that Aspen HYSYS modeling and simulation can contribute to some aspects of the customization requirements as listed earlier in this presentation, while the rest can be addressed from laboratory analysis and formulations.

The identified reactions were modelled in varied layers of complexities in Aspen HYSYS: steady state, sensitivity analysis, optimization and transient conditions in a CSTR at varied reaction conditions and time to produce varied esters properties.

9. Conclusion

The advanced Aspen HYSYS modelling of different complexities of hierarchical layers of simulation aimed at customizing esters derived from palm oils for different application has fully demonstrates the reliability and flexibility of the models. The results show that further customization of esters using this model can be realized by applying various kinetic and process parameters, and imposing appropriate constraints on the model. Results from the models demonstrate the reliability of the various layers of the complexities of the simulation; show properties of the esters at various process conditions and therefore reveals prospects for customizing these esters derived from the transesterification of palm oils for various applications. Overall, the results show that this approach can guide further laboratory and modelling research towards customizing palm oil as drilling fluid additive.

Figure-4. Flowsheet representation of the Aspen HYSYS model

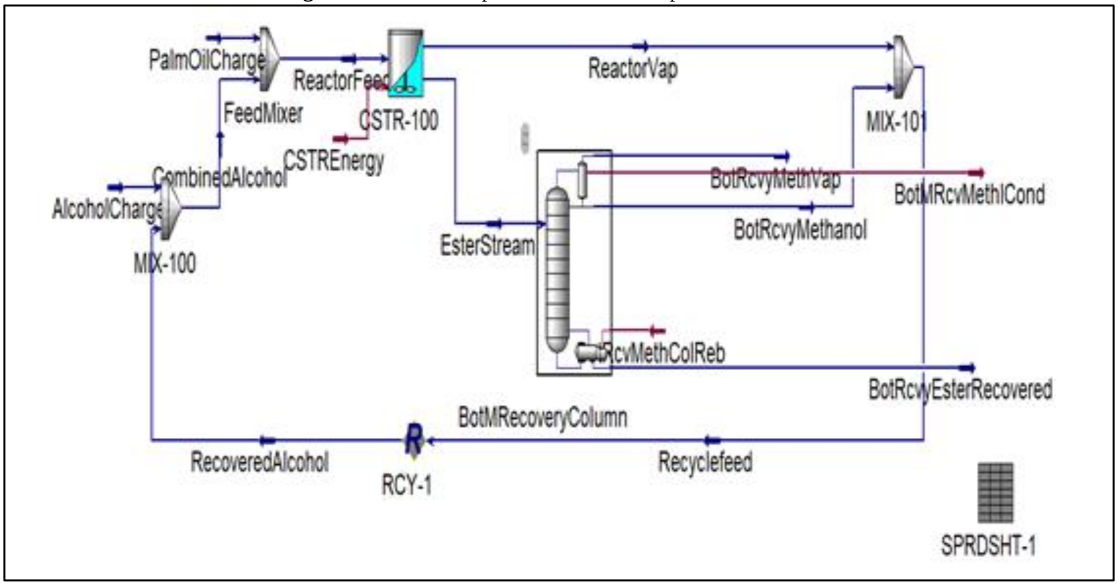


Table-5. Steady State sensitivity analysis at various conditions

Reactor Volume (Litre) **30**

	Reaction Extent (HYSYS) 1	2	3	*Res Time min*	*Bulk LiqTemp C*	*Ester Viscsity Index*	*Ester Purity*	*Ester Mol Weight*	*Ester Desity kg/m3*	*Ester Viscsity cp*
5	16.81	11.77	11.24	1.45	147.90	0.20	0.70	272.20	797.90	0.65
6	14.10	11.51	11.20	1.68	127.70	5.00	0.76	244.70	807.60	0.92
7	12.01	10.79	10.61	1.89	114.30	7.33	0.79	223.20	815.80	1.12
8	10.51	9.95	9.85	2.09	104.20	8.31	0.81	204.50	822.20	1.23
9	9.34	9.11	9.05	2.28	96.62	8.41	0.81	187.90	827.20	1.25
10	8.41	8.35	8.32	2.46	90.90	8.01	0.81	172.70	830.70	1.21

Reactor Volume (Litre) **80**

APO	*Reaction Extent (HYSYS)* 1	2	3	*Res Time min*	*Bulk LiqTemp C*	*Ester Viscsity Index*	*Ester Purity*	*Ester Mol Weight*	*Ester Desity kg/m3*	*Ester Viscsity cp*
5	16.81	15.02	14.90	3.86	139.10	5.12	0.80	243.10	797.60	0.92
6	14.10	13.25	13.21	4.47	124.80	7.36	0.83	228.20	806.90	1.12
7	12.01	11.81	11.80	5.05	113.20	8.65	0.84	213.30	814.80	1.26
8	10.51	10.57	10.61	5.59	103.90	9.12	0.84	198.70	821.30	1.32
9	9.34	9.52	9.52	6.09	96.65	8.99	0.84	184.30	826.40	1.32
10	8.41	8.64	8.70	6.57	91.04	8.46	0.83	170.50	830.10	1.26

Figure-5. Sensitivity analysis for key kinetics parameters

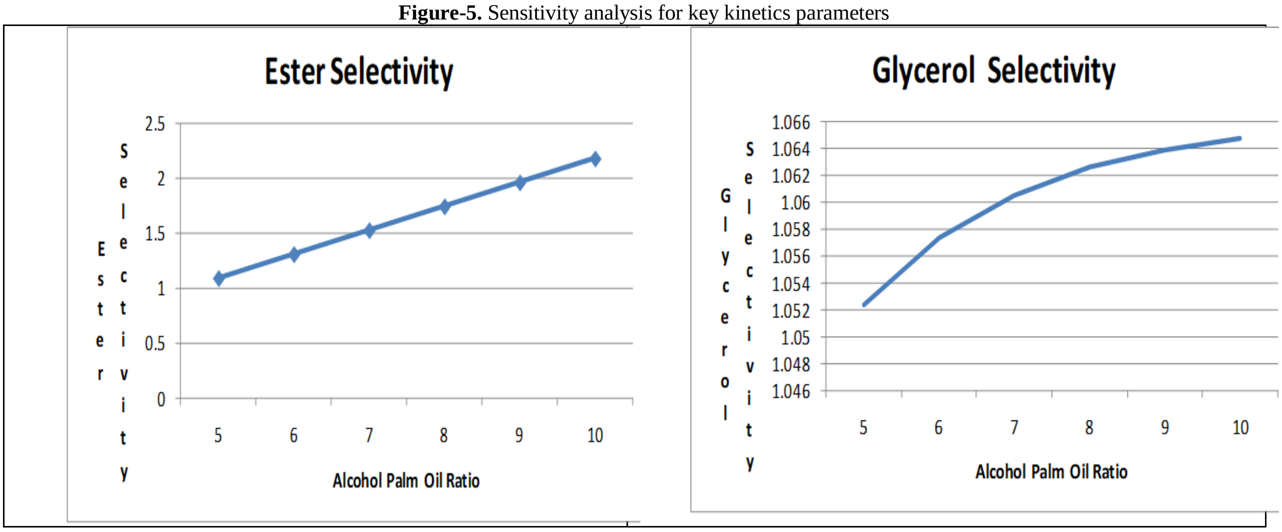
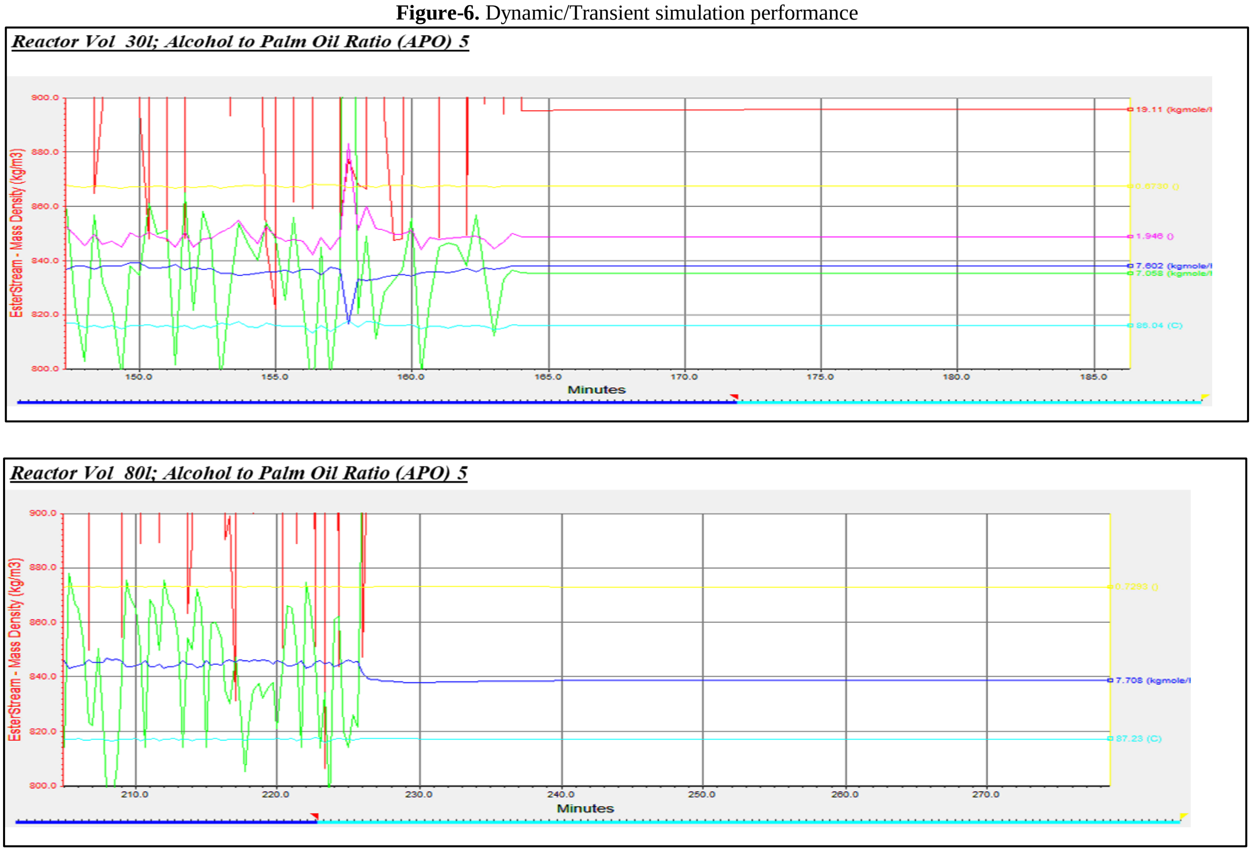


Figure-6. Dynamic/Transient simulation performance



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