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Novel De-Oiling of Oil-Water

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Abstract: The study anchors on developing a mechanistic model for oil-water separation. Over the years, researchers have been working on how to improve the quality of produced water effluent especially from oil and gas operations sent to the receiving waters. Despite the standard set for compliance by regulatory bodies like united nation agency, ministry, departments and other agencies both state and federal government including non governmental agencies the problem of meeting stipulated bench marks still persist. This study however looks into some variables perceived as being relative to improving or affecting produced water effluent from oil-water separator. Modeling of oil-water separation was based on the philosophy that a mathematical model can be established for the physical problems under investigation. These mathematical problems formulated were based on laws of conservation. Solving the model equation analytically however pose some problems. Hence they were solved by simulation using a computer soft ware SIMULINK a graphical extension of MATLAB with positive outcome since it has the ability to model non-linear systems. From the simulated analysis, increased flow rate creates turbulence in the system with resultant poor effluent quality, whereas also, from the simulated analysis, gradual increases in temperature improves oil-water separation from lower temperature of the fluid upstream thereby aiding improvement in effluent quality.

Keywords: Mass, Energy, Simulink, Concentration, Flow Rate, Temperature

Introduction

Petroleum is vital to many industries and in the manufacture of a wide variety of materials. It also accounts for a large percentage of the world’s energy needs and thus it is a critical concern for many nations (Shahryar, 2017). Wastewater or oil-water effluent management practices can be implemented by prevention (improved operation or operating procedures), source reduction or waste minimization (material elimination, inventory control and management, material substitution, process and equipment modifications), reuse, recycling/recovery, treatment and disposal. Setting and enforcing environmental regulations in the oil and gas industry are important for minimizing potential environmental impacts and protecting human health and the environment (Shahryar, 2017). The function of an oil production facility is to separate the oil well stream into three components or phases (oil, gas and water) and process these phases into some marketable products or dispose of them in an environmentally acceptable manner (Sayda and Taylor, 2007). The major research task of modeling oil-water separation involved, constructing and simulating flow in the paradigm. The physical model constructed with Perspex glasses about 5mm in thickness also included the internals like baffles and the hydraulic weir. However, the gravity settling approach requires very long cylinder which is not practical and inconsistent with space restriction in the laboratory (Kharoua et al., 2013). Produced water is the largest waste stream generated in oil and gas industries. It is a mixture of different organic and inorganic compounds (Fakhrul-Razi et al., 2009). Modelling of oil-water separation might not be new. However, a model may be seen as a description of a system using mathematical concepts and language. Hence this would metaphor into a statement of an equality containing one or more variables called equations. This study is expected to improve on mathematical formulation describing oil-water separation due to high cost of improving produced water treatment through chemicals. This study might also help explained liquid-liquid separation in a gravity vessel both analytically and the effect of different components. If this is achieved, the study would impart positively or
benefit oil and gas industries in terms of optimization of oil production, reduction in pollution of receiving waters, produced water re-injection, design and cost reduction in terms of produced water treatment. Utilities companies, water treatment entities including the academia and the reading public are not left out as direct beneficiaries of this study.

Aim and Objectives

The aim of this research is the formulation, solution and simulation of mathematical relationships describing oil- water separation.

Methodology

In developing a mathematical model for the multiphase oil-water separation, the following assumptions were adopted for the mechanistic model:

a. The fluid particles are spherical in size
b. The dynamics of gas phase ignored
c. The mode of separation of the liquid particles is not hindered.
d. The pressure of the two liquid in the vessel are not equal.
e. The holding tank is assumed to be the reservoir
f. Perfect mixing.
g. Mass and concentration density \( C_{\rho} \) are constants.
h. Exothermic first order reaction.
i. Perfectly insulated (no heat loss).
j. Water is the continuous phase and oil is the dispersed phase.
k. Smooth interface and smooth vessel wall
l. Negligible surface energy between vessel wall and fluid
m. Homogenous dispersion.
n. Steady state flow.
o. Density of the two liquid are different.

Applying the basic principles of conservation of mass in the first instance which states that for any system closed to all transfer of matter and energy, the mass of the system must remain constant over time. The model under study, where the total mass and energy cannot be generated neither do they disappear, so that mass balance would give a differential equation which is ordinary. This ordinary differential equation contains one or more functions of one independent variable and its derivatives. The equation relates some functions with it derivatives. These functions which are physical quantities include, concentration, flow rate, mass, density, velocity, area, temperature etc. While the derivative would represent the rate of change and the equation to be derived would define the relationship between the two. For example the Equation (2.1) (Luyben, 1990):

\[
\frac{dM}{dt} = \sum \rho_i F_i - \sum \rho_j F_j
\]  

(2.1)

where, \( \rho_i, \rho_j \) are the densities of inlet and outlet streams; \( F_i, F_j \) are volumetric flow rates of the inlet and outlet streams. However, the differential equation will accompany set of additional constraints called boundary conditions:

\[
\frac{dM}{dt} = F_i \rho_i - F_o \rho_o
\]  

(2.2)

\[
\rho = \frac{M}{V}
\]  

(2.3)

where, \( M, \rho, V \) is the Mass, Density and Volume; \( F_i, F_o \) are the mass flow rate of oil and water inlet, outlet streams.

Substituting Equation (2.3) into Equation (2.2) we have:

\[
\frac{d(\rho V)}{dt} = F_i \rho - F_o \rho
\]  

(2.4)

where, \( \rho \) is the density of liquid stream which is assumed constant.

Hence we obtain:

\[
\frac{dV}{dt} = F_i - F_o
\]  

(2.5)

However in developing the mathematical relationship for oil/water separation, what is paramount here is the degree of concentration in terms of component species. Hence the lower the component species in terms of concentration the better the quality of the produced water. This led to introduction of concentration into Equation (2.5) through the overall mass balance Equation (2.6).

Overall Mass Balance:

\[
\frac{\text{Rate of Mass Accumulation}}{\text{Mass Input}} - \frac{\text{Rate of Mass Output}}{\text{Mass Input}} = \frac{\text{Rate of Generation}}{\text{or Depletion of Component A}}
\]  

(2.6)

However, the accumulation term will supply the time derivative and produce a differential equation.

Component mass balance gives:

\[
\left( \frac{\text{Rate of Accumulation}}{\text{of Component A}} \right) = \left( \frac{\text{Rate of Input}}{\text{of Component A}} \right) - \left( \frac{\text{Rate of Generation}}{\text{or Depletion of Component A}} \right) - \left( \frac{\text{Rate of Output}}{\text{of Component A}} \right)
\]

Hence, we have:
\[ \frac{dV}{dt} = [F_A(C_A - (-r_A))V - F_C A] \]  
(2.7)

Applying Product Rule to Equation (2.7) we have:

\[ C_A \frac{dV}{dt} + V \frac{dC_A}{dt} = F_C A + F_C A - (-r_A)V \]  
(2.8)

where, \((-r_A) = \text{Rate of Disappearance of component } A.\)

Simplifying, we have:

\[ C_A(F_A - F_A) + V \frac{dC_A}{dt} = F_A C_A - F_A C_A - (-r_A)V \]  
(2.9)

Collecting like-terms, we have:

\[ V \frac{dC_A}{dt} = F_A(C_A - C_A) - (-r_A)V \]  
(2.10)

Dividing throughout by Volume, \(V\), we have:

\[ \frac{dC_A}{dt} = \frac{F_A}{V}(C_A - C_A) - (-r_A) \]  
(2.11)

where, \(\text{`r' = rate of disappearance of component } A \text{ or reaction rate.}\) The reaction rate expression used in dynamic modeling are typically based on the principles of mass action (Luyben, 1990). Hence Arrhenius expression must be incorporated when rate constants depend on temperature, otherwise, the energy balance will not adequately describe temperature change. Hence Arrhenius Equation (2.12) state as follow:

\[ -r_A = Ke^{-E/RT}C_A \]  
(2.12)

Where:

\( R = 8.314 \text{ J/K.mol} \)
\( T = \text{Temperature in Kelvin} \)
\( e = \text{Euler’s number} = 2.71828 \)
\( A = \text{Represents and is dependent on collision frequency} \)
\( E_A = \text{Actuation energy require for separation to take place} \)

The description of the above equation resulted in the establishment of the first equation for the model:

\[ \frac{dC_A}{dt} = \frac{E}{V}(C_A - C_A) - KCT e^{-E/RT} \]  
(2.13)

Furthermore, another equation was also formulated still from the law of conversation that is for total energy balance. It states that the total energy of an isolated system remains constant and it is said to be conserved overtime (Luyben, 1990).

\[ \frac{dE}{dt} = \frac{d(U + K + P)}{dt} = \sum \rho_j F_j h_i - \sum \rho_j F_j h_j \]  
(2.14)

Where:

\( E = \text{The total energy content} \)
\( U = \text{The internal energy} \)
\( K = \text{The kinetic energy} \)
\( P = \text{The potential energy} \)
\( h_i, h_j = \text{The enthalpies of inlet and outlet streams} \)

Though for fluid system the potential, kinetic energy are usually negligible:

- That is \( \frac{dk}{dt} = \frac{dp}{dt} = 0 \)
- Hence \( \frac{dU}{dt} = \frac{dH}{dt} \)

where, \( H = \text{the total enthalpy of the liquid} \):

\[ \frac{dH}{dt} = F_j h_i - F_j h_j \]  
(2.15)

where, \( h_i, h_o = \text{the specific enthalpies of water, oil and inlet oil/water respectively} \):

\[ B = H = C_p M T \]  
(2.16)

And \( \rho = \frac{M}{V} \), substituting into Equation (2.16), we have:

\[ H = C_p T \rho V \]  
(2.17)

Also considering the concentration of the produced water in terms of component species, we equally introduce
the component energy balance. This is the first law of thermodynamics which states that for any bounded system.

Energy In – Energy Out across the boundaries = Energy accumulated inside the boundaries.

Using this definition, we can easily express the rate of temperature change in a insulated system/vessel as a function of mass flow through the tank, the fluid heat capacity, density and tank volume.

Component energy balance state as follows:

\[
\frac{dV}{dt} \rho C_p \frac{dT}{dt} = F_i \rho C_p T_i - F \rho C_p T - Q + (-\Delta H)(-r_a)V 
\]

\[\text{(2.19)}\]

Where:

- \( F_i \) = Inlet flow rate
- \( \rho \) = Density
- \( C_p \) = Inlet heat capacity
- \( T_i \) = Inlet temperature
- \( F \) = Outlet flow rate
- \( T \) = Outlet temperature
- \( V \) = Volume of liquid
- \( (-\Delta H) \) = Energy added
- \( Q \) = Energy removed

By applying product rule principles, we have:

\[
V \frac{dT}{dt} + T \frac{dV}{dt} = F_i T_i - F T - \frac{Q}{\rho C_p} + \frac{(-\Delta H)(-r_a)V}{\rho C_p} 
\]

\[\text{(2.20)}\]

\[
V \frac{dT}{dt} + T (F_i - F) = F_i T_i - F T - \frac{Q}{\rho C_p} + \frac{(-\Delta H)(-r_a)V}{\rho C_p} 
\]

\[\text{(2.21)}\]

\[
V \frac{dT}{dt} = F_i (T_i - T) - \frac{Q}{\rho C_p} + \frac{(-\Delta H)(-r_a)V}{\rho C_p} 
\]

\[\text{(2.22)}\]

\[
\frac{dT}{dt} = \frac{F_i}{V} (T_i - T) - \frac{Q}{V \rho C_p} + \frac{(-\Delta H)(-r_a)}{\rho C_p} 
\]

\[\text{(2.23)}\]

We already know the Arrhenius equation which can be substituted into Equation (2.23)

Hence, we have as shown in Equation (2.24) the second model equation:

\[
\frac{dT}{dt} = \frac{F_i}{V} (T_i - T) - \frac{Q}{V \rho C_p} + \frac{(\Delta H)K C e^{-E/RT}}{\rho C_p} 
\]

\[\text{(2.24)}\]

\[
\frac{dT}{dt} = \frac{F_i}{V} (T_i - T) - \frac{Q}{V \rho C_p} + \frac{(\Delta H)K C e^{-E/RT}}{\rho C_p} 
\]

\[\text{(2.25)}\]

**Results and Discussion**

Simulation was carried out by varying the Inputs concentration from 0.25-1.0 mg/l.
Fig. 2: Shows component mass balance flow chart

Fig. 3: Component mass balance/Arrhenius

For the simulation, the following variables were kept constant before varying input concentration.

Fluid volume = 5,000-20,000 bbl or 1 m$^3$, Inlet Temperature from 293 k, Input concentration = 0.05 kg/m$^3$, Integrator = 1, $K_0 = 0.001$ m$^{-1}$s$^{-1}$, $E = 1.6*10^5$ J/mol, $R = 8.314$ J/mol-k, $Q = 15$ m$^3$/s, Component density = 1000 kg/m$^3$, Specific heat at constant pressure = 20.8 J/mol.k.

Simulation was carried out by varying the Inputs Volumetric Flow Rate from 0.01-25.0 m$^3$/s.

However, every other parameter was kept constant including the units. Fluid volume = 10,000-20,000 bbl or 1 m$^3$, Input concentration = 0.00035 kg/m$^3$, Integrator = 1, $K_0 = 0.001$ m$^{-1}$s$^{-1}$, $E = 1.6*10^5$ J/mol, $R = 8.314$ J/mol-k, Inlet temperature in Kelvin = 298k, $Q = 20$ m$^3$/s, Component density = 1000 kg/m$^3$, Specific heat at constant pressure = 20.8 J/mol.k.

Simulation was carried out by varying Inlet Temperature from 293-450 k.
Fluid volume = 10,000-20,000 bbl, Input concentration = 0.00035 kg/m$^3$, Integrator = 1, $K_0 = 0.001$ m$^{-1}$s$^{-1}$, $E = 1.6 \times 10^3$J/mol, $R = 8.314$J/mol-k, $Q = 15$ m$^3$/s, Component density = 1000 kg/m$^3$, Specific heat at constant pressure = 20.8 J/mol.k.

However, the two model Equations (2.13), (2.25) were solved by simulation using Simulink a graphical extension of MATLAB software since it has the ability to model non-linear system and the ability to take on initial conditions. From Fig. 1 to 4 it was seen that from the simulation according to the first model equation there were responses in the $C_A$-value representing the outlet concentration that is the effluent. This was achieved by keeping other variables constant and varying a particular parameter one at a time like, the retention time, flow rate, sample volume, temperature, etc. For example, increasing flow rate creates turbulence with resultant poor effluent quality. In the course of simulating with the software, input values ranges between plus and minus. This was geared towards improving the effluent quality at a particular set value from the micro model and comparing it with a macro system. This in turn verified the fact that results were in agreement with the macro results that varying the variables actually influences oil-water separation effluent quality. That is at certain set values considering the variables in model Equation (2.13) and Equation (2.24) the produced water or effluent quality can greatly be improved if applied.

![Energy balance flow chart](image1.png)

**Fig. 4:** Shows energy balance flow chart

![Input concentration output response](image2.png)

**Fig. 5:** Shows input concentration @ 1.0 mg/l output response.
Fig. 6: Shows input concentration @ 0.25 mg/l output response.

Fig. 7: Shows input volumetric flow rate @ 15 m³/s output response

Fig. 8: Shows input volumetric flow rate @ 25 m³/s output response.
However Fig. 5 shows the effluent quality from output response during simulation which was time dependent. At a concentration of 1.0 mg/l, there was a steady profile for a long while before the curve started declining. Whereas Fig. 6 with reduced concentration of 0.25 mg/l with same simulation time, a far more quality effluent was achieved.

We also observed that increasing the volumetric flow rate creates turbulence in the system hence resulting in decreasing effluent quality. Figure 7 shows a more prolong time in the gravity separation since retention time is a major determinant in oil-water separation hence improved produced water. Whereas, Fig. 8 shows a short time response which inevitably leads to poor separation.

Furthermore, Fig. 9 shows the effect of increasing temperature on oil-water separation from 450 k. The produced water quality shows a significant improved quality considering the same time duration as compared with that in Fig. 10 at a temperature of 350 K.

**Conclusion**

The simulation from the Simulink software an extension of MATLAB using the model equations shows, how the variables of temperature, volumetric flow rate, sample concentration affects, influences oil-water effluent or produced water from oil and gas industries. This work is in agreement with the work of (Abdulkadir and Hernandez-Perez, 2010) where CFD
was used in simulating the effect of flow rate, oil droplet diameter on separation efficiency.

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**Author’s Contributions**

All authors equally contributed in this work.

**Ethics**

This article is original and the authors declare their responsibility for any ethical issues that may arise in the course of publication of this manuscript.

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