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# Modeling of chemical processes using commercial and open-source software: A comparison between Aspen Plus and DWSIM

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**Abstract.** Computer simulation plays a key role in chemical process design. Currently, there are a large number of widely accepted commercial software. For example, Aspen Plus which was used to simulate offshore petroleum production processes, but it is often too costly to purchase and maintain a valid software license. On the other hand, since open-source software is freely accessible, the simulation models developed using open-source software could be studied, reviewed, and modified by any interested parties. This would help promoting technology transfer and knowledge dissemination in both academic and industry sectors. We specifically focus on the simulation of chemical process using the modeling software to evaluate thermal and chemical behaviour of the system which uses the chemical processes related to offshore petroleum production facilities as an example to demonstrate the software capabilities of both Aspen Plus and DWSIM. This work emphasizes on the comparison of simulation results calculated by commercial software namely Aspen Plus vs. open-source software called DWSIM (An open-source sequential modular steady state simulator) [1]. The simulation was carried out under the steady-state conditions, adiabatic processes, and negligible pressure losses. Finally, simulation results from DWSIM and Aspen Plus were compared with the heat and mass flow diagram which was used as reference. It was found that the discrepancy between simulation and reported values was in general less than 5%. It has been demonstrated that free and open-source software like DWSIM could potentially perform similar tasks as commercial software.

**Keywords:** Chemical Process modeling, Offshore petroleum, Aspen Plus, DWSIM

## 1. Introduction

Nowadays simulation plays a crucial part in various engineering-related problems. There are plenty of commercial software packages available. Some of them are free such as DWSIM, HYDROFLO and OpenModelica [1], while the others can be purchased from the market such as ASPEN Plus, ASPEN HYSYS, ProSim Plus, and UniSim software [2]. Open-source research software is becoming



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increasingly common in the chemical process modeling community [3]. Hence, it is possible to investigate the behavior of pilot plants using a computer simulation without having to conduct experiments so that the experimental cost can be significantly reduced. Aspen Plus and DWSIM are of particular interest in this work. Aspen Plus is widely accepted commercial software that could be used to simulate offshore petroleum production processes to assess the quantity and feasibility of waste heat recovery. Although it is high capability of modeling complex chemical processes involving various chemical reactions and substances with substantial validation databases and professional software support, Aspen Plus is necessary to purchase and maintain a valid software license. In addition, simulation models created from commercial software would have to be opened, modified and run using the software itself; exporting the models to any other software could not be easily implemented due to various issues such as proprietary file formatting, and data compression algorithms. Such restrictions could hinder research collaboration involving various organizations in order to work on previously developed process models, they would have to first purchase the software. DWSIM is an open-source chemical process simulation which was created by Daniel Medeiros. DWSIM allows user to better understand the behavior of chemical systems with no cost as it is freely accessible [4]. Aspen plus is widely accepted commercial software which relies on process simulators built from over 35 years of experience and feedback from top chemical companies [5]. The objective of this study is to evaluate the modeling capability of DWSIM, a free open-source software, by comparing the simulation results with those obtained from commercial software i.e. Aspen Plus. In this work, offshore petroleum production facilities were used as an example to demonstrate the simulation capability of both DWSIM and Aspen Plus. Booster Compression and Sale Gas Compression were chosen as representative processes to be studied in this work. Booster Compression, one of the main systems, is used to pressurize gas products. The Booster Compression receives the gas products from previous processes involving the separation of gas products, from condensate and unwanted impurities out of the feed streams. After the gas compression, then the gas products will be sent to Carbon Dioxide (CO<sub>2</sub>) Removal and Sales Gas Compression processes respectively. CO<sub>2</sub> Removal is performed as a filtering process that takes out the unwanted CO<sub>2</sub> from the gas products. After this process, the gas pressure will decrease, thus it will be necessary to use Sale Gas Compression to increase the pressure again after the CO<sub>2</sub> Removal process. Sales gas compression process is also used to pressurize the gas for exporting from offshore platform via transmission pipe to onshore distribution stations.

### Nomenclature

$\dot{E}$	Energy (kW)		
$\dot{Q}$	Heat transfer rate (kW)	$h$	Enthalpy (kJ/kg)
$\dot{W}$	Mechanical Power (kW)	$P$	Pressure (N/m <sup>2</sup> )
$\dot{m}$	Mass flow rate (kg/s)	$R$	Universal gas constant (J K <sup>-1</sup> mol <sup>-1</sup> )
$A_v$	Velocity of system (m/s)	$V$	Volume (m <sup>3</sup> )
$g$	Gravitational acceleration (m <sup>2</sup> /s)	$T$	Temperature (K)
$z$	Hight base on datum (m)	$\omega$	acentric factor

## 2. Theory

### 2.1 First Law of Thermodynamic

Energy can be converted from one form to another, but it cannot be created nor destroyed, under any

circumstances. Mathematically, this is represented as  $\dot{E}_{in} - \dot{E}_{out} = \frac{dE_{sys}}{dt}$

Energy balance for steady flow [6];

$$(\dot{Q}_{net,in}) - (\dot{W}_{net,out}) = \sum_{out} \dot{m}(h + \frac{1}{2}v^2 + gz) - \sum_{in} \dot{m}(h + \frac{1}{2}v^2 + gz) \quad (1)$$

Neglecting the change in potential and kinetic energy, the energy equation becomes;

$$(\dot{Q}_{net,in}) - (\dot{W}_{net,out}) = \dot{m}(\sum_{out} h - \sum_{in} h) \quad (2)$$

### 2.2 Peng-Robinson equation of state

Peng-Robinson equation of state is the model for thermodynamic and volumetric calculations which is applied in this simulation. Equations are represented as [7]

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m^2 + 2bV_m - b^2} \quad (3)$$

$$a \approx 0.45724 \frac{R^2 T_c^2}{P_c} \quad (4)$$

$$b \approx 0.07780 \frac{RT_c}{P_c} \quad (5)$$

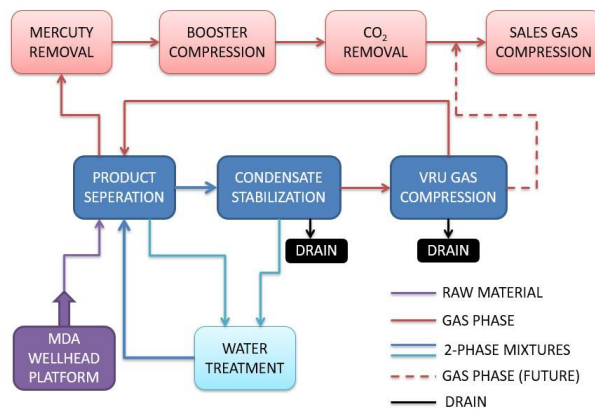
$$\alpha = \left[ 1 + k \left( 1 - T_r^{1/2} \right) \right]^2 \quad (6)$$

$$k \approx 0.37464 + 1.5422\omega - 0.26992\omega^2 \quad (7)$$

$$T_r = \frac{T}{T_c} \quad (8)$$

### 3. Methodology

The offshore petroleum production process is consisting of 9 modules as shown in Figure 1. The raw petroleum is pumped by wellhead platform and is separated to gas phase and liquid phase by product separation. Gas phase is transported to mercury removal for decomposing mercury before being sent to booster compression to increase pressure. After that CO<sub>2</sub> will be removed from the gas at CO<sub>2</sub> Removal. Then, the gas will be pressurized at sale gas compression and proceed to metering station, transmission pipeline, and to onshore distribution stations. Liquid phase is separated at production separation, delivered to condensate stabilization and VRU (vapor recovery unit) gas compression to condense hydrocarbon vapor to liquid and recirculate it back to the product separation.



**Figure 1.** Plant flow diagram of offshore petroleum production process.

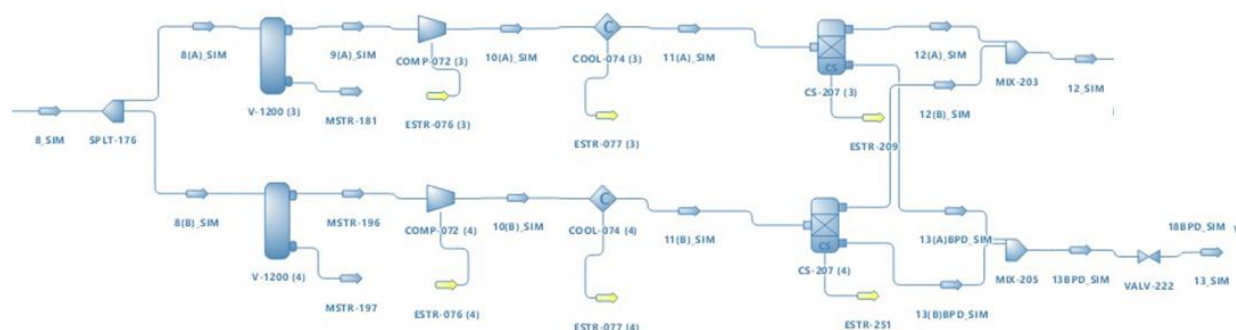
In this work, we will focus on the Booster Compression and Sales Gas Compression processes.

### 3.1 Booster Compression

Before the gas products enter the CO<sub>2</sub> removal process, gas pressure needs to be increased because a large pressure drop will occur while extracting CO<sub>2</sub> out of the gas. There are 4 main devices in the Booster Compression: Suction Scrubber, Compressor, Discharge Cooler [5] and Discharge Scrubber. Splitter and Mixer are also inserted into the model flowsheet.

#### 3.1.1 Simulating Booster Compression by using DWSIM

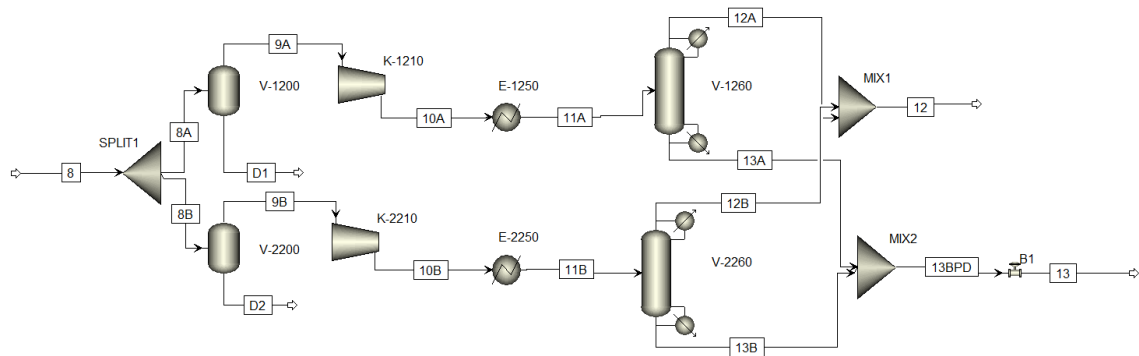
Pre-processing step may begin by clicking “New steady state simulation” then selecting the compound and property packages. In this case, the Peng-Robinson equation of state was chosen. This equation of state is suitable for hydrocarbon compound. Next, relevant process equipment is connected to form a flowsheet as shown in Figure 2. Appropriate initial conditions must be specified so that the flowsheet can be computed. The calculation can be performed by clicking “Solve flowsheet” (F5) for processing step. Finally, insert “Master Property Table” to view the simulation result.



**Figure 2.** Booster Compression Model in DWSIM.

#### 3.1.2 Simulating Booster Compression by using Aspen Plus

Pre-processing begins by clicking at the Properties tab and then Component tab to insert chemical composition of working fluid of interest. In this work, the working fluid is a mixture of various substances ranging from light to heavy hydrocarbon plus some impurities such as Mercury, Carbon dioxide, Hydrogen sulfide, etc. Next, the method for thermodynamic property evaluation must be specified. In this work, the Pen-Robinson equation of state was chosen as it has been commonly used when analyzing hydrocarbons. Then, process equipment of the Booster Compression has been placed and linked in a sequential order according the underlying process flow diagram as shown in Figure 3. The initial conditions must also be specified by filling in the fraction of each component at input node as well as the initial pressure, temperature, and mass flow rate. Once the necessary initialization is complete, the flowsheet calculation may proceed by clicking at the Run button. For the post-processing step, the simulation result can be examined by selecting the stream result where various properties of all nodes in the flowsheet are summarized in one table including temperature, pressure, enthalpy, mole fraction, etc.



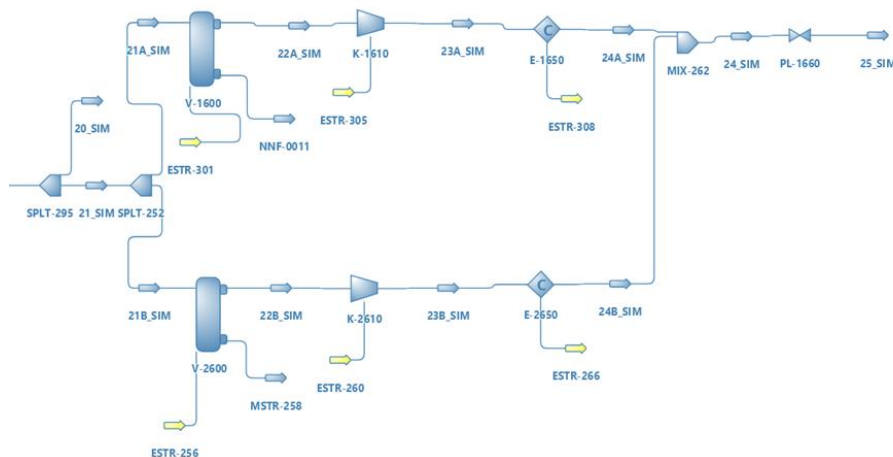
**Figure 3.** Booster Compression Model in Aspen Plus.

### 3.2 Sales Gas Compression and Export

Sales Gas Compression and Export is the final process of natural gas production in offshore platforms. It is used to increase the gas pressure after the CO<sub>2</sub> removal process and to overcome the pressure drop while being transported to metering stations, transmission pipeline and distribution stations onshore. There are 4 devices in this process module comprising Suction Scrubber, Compressor, Discharge Cooler and Pig Launcher [6]. The procedures for process flowsheet creation, parameter initialization and flowsheet calculation are the same as those described in Booster Compression section. The process flowsheet of Sales Gas Compression in DWSIM and Aspen Plus are shown in Figures 4 and 5, respectively.

#### 3.2.1 Simulating Sales Gas Compression and Export by using DWSIM

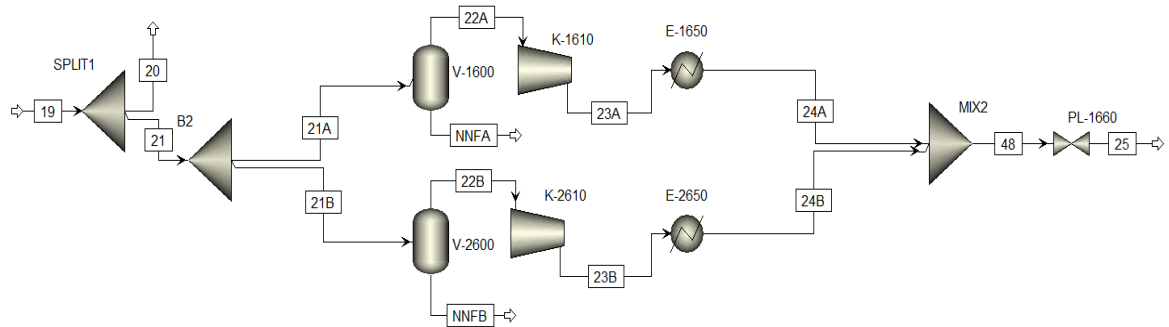
Simulation procedures are essentially similar to those described in Section 3.1.1. Process equipment includes Suction Scrubber, Compressor, Discharge Cooler, Mixer, Splitter and Valve. The major difference between Booster Compression and Sales Gas Compression are the operating pressure, temperature, and chemical composition of gas products. The flowsheet of Sales Gas Compression and Export in DWSIM is shown in Figure 4.



**Figure 4.** Process equipment of Sales Gas Compression and Export in DWSIM.

#### 3.2.2 Simulating Sale Gas Compression and Export by using Aspen Plus

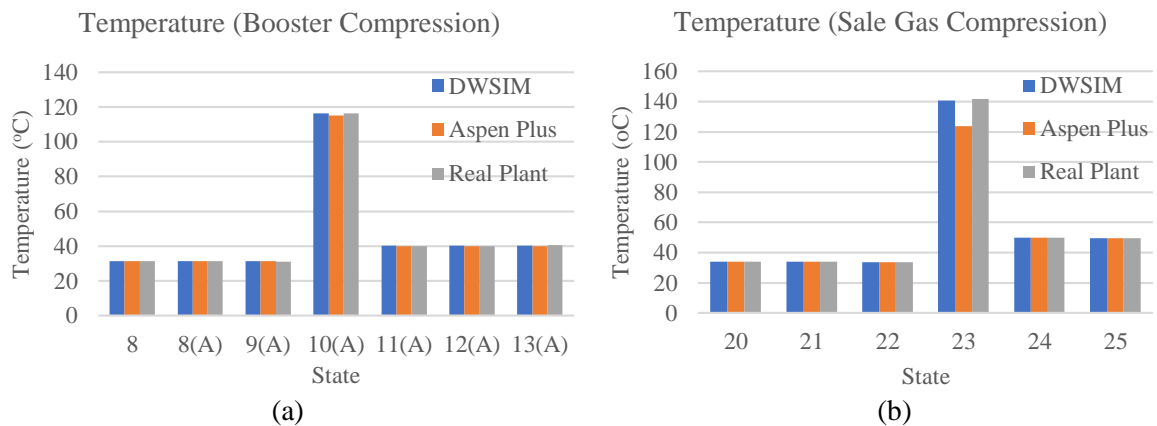
To create the Sales Gas Compression and Export model in Aspen Plus, the simulation procedures are generally the same as what was described in Section 3.1.2. The flowsheet corresponding to Sales Gas Compression and Export in Aspen Plus is show in Figure 5.



**Figure 5.** Process equipment of Sales Gas Compression and Export in Aspen Plus.

#### 4. Results and discussion

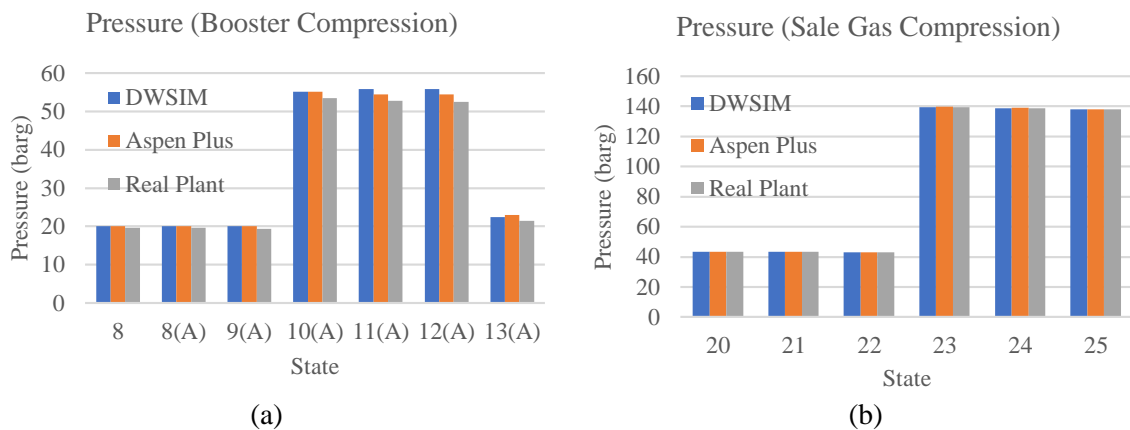
Following flowsheet calculation in both DWSIM and Aspen Plus, the accuracy of simulation results could be evaluated based on plant's heat and mass flow diagram. The parameters of interest include temperature, pressure, mass flow rate, and chemical composition of the gas products. Figure 6 compares simulation results from DWSIM and Aspen Plus with reported values from Real Plant. Generally, they are in an excellent agreement between the calculated and reported values. In both Booster Compression and Sales Gas Compression modules, the difference is less than 1% in almost all states except at the State 23 as calculated by Aspen Plus. In this case, the error in temperature is 12.733% which may have originated from different computational methods and assumptions between these two codes.



**Figure 6.** Comparison of temperature of each state for (a) Booster Compression (b) Sales Gas Compression.

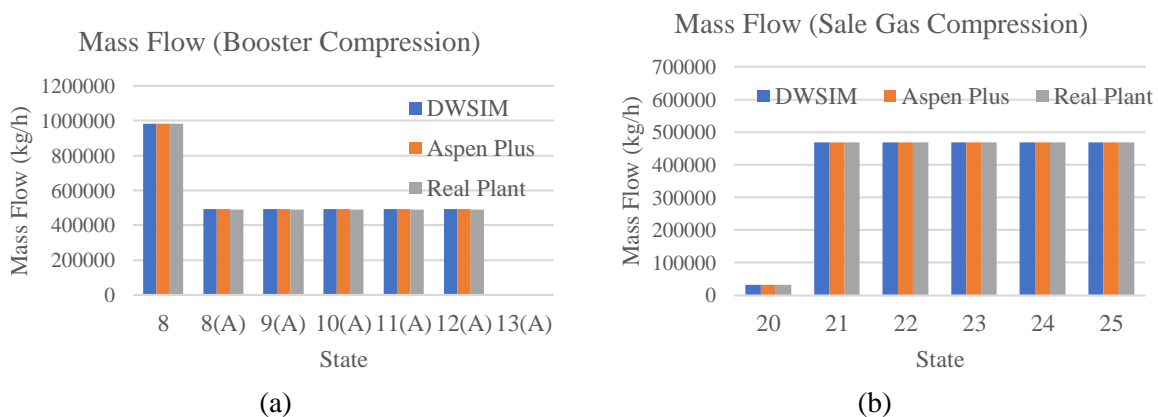


In case of the pressure of each state, Figure 7 compares the simulation results from DWSIM and Aspen Plus with reported values from HMB. Again, they agree quite well except for certain states. In this case, it was observed that the maximum deviation occurs at State 13A as calculated by Aspen Plus by 7.771%. State 13A is the state from which the gas products leave compound separator. This state had slightly more deviation than others as DWSIM predicted this state as liquid while Aspen Plus predicted it as vapor. Therefore, the predicted density and volumetric flow rate from DWSIM and Aspen Plus were significantly different. Anyway, difference in density did not greatly affect the pressure calculation as the difference between DWSIM and Aspen was less than 1%.



**Figure 7.** Comparison of pressure of each state for (a) Booster Compression (b) Sale Gas Compression.

For mass flow rate, the deviation between calculated and reported values is very small as shown in Figure 8 for most states except for the state 13A, which was predicted as liquid by DWSIM and vapor by Aspen Plus. At this state, the difference between simulation results and reported values was 6.37% for DWSIM and 18.50% for Aspen Plus, respectively. These errors may have come from the accumulation of small deviation in previous state. Nevertheless, the flow rate of State 13A is insignificantly small when compared to that of other states, thus, the deviation can be negligible.



**Figure 8.** Comparison of mass flow rate of each state for (a) Booster Compression (b) Sale Gas Compression.



The next parameter to be examined is the chemical composition of the gas products. In fact, there are more than 20 chemical species contained in the gas products. From brevity, only chemical substances with mole fraction greater than 1% are reported which are Carbon dioxide, Water, Nitrogen, Methane, Ethane, Propane, Isobutane, N-butane. The other components that have not shown in this paper are neglected because their mole fractions are too small.

Table 1 show the relative error of chemical composition as calculated by DWSIM when compared to real plant data. It can be noticed that the relative errors are less than 2% except for water vapor which is about 5%. However, the relative error for the State 13(A) is slightly higher than other states. This may have been because there are higher uncertainties involved when dealing with condensation process.

**Table 1.** Chemical composition of each state for Booster Compression as calculated by DWSIM and the relative error when compared with reported values from heat and mass flow diagram.

Component	DWSIM							Relative error (%)						
	8	8(A)	9(A)	10(A)	11(A)	12(A)	13(A)	8	8(A)	9(A)	10(A)	11(A)	12(A)	13(A)
Carbon dioxide	0.45	0.45	0.45	0.45	0.45	0.45	0.01	0.07	0.07	0.07	0.07	0.07	0.07	1.43
Water	0.00	0.00	0.00	0.00	0.00	0.00	0.99	5.06	5.06	5.06	5.06	5.06	4.77	0.01
Nitrogen	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.28	0.28	0.28	0.28	0.28	0.28	1.69
Methane	0.45	0.45	0.45	0.45	0.45	0.45		0.24	0.24	0.24	0.24	0.24	0.24	
Ethane	0.05	0.05	0.05	0.05	0.05	0.05		0.08	0.08	0.08	0.08	0.08	0.08	
Propane	0.03	0.03	0.03	0.03	0.03	0.03		0.24	0.24	0.24	0.24	0.24	0.24	
Isobutane	0.01	0.01	0.01	0.01	0.01	0.01		0.65	0.65	0.65	0.65	0.65	0.65	
N-butane	0.01	0.01	0.01	0.01	0.01	0.01		0.87	0.87	0.87	0.87	0.87	0.88	

Table 2 reports similar results as in Table 1 but the reported values were calculated by Aspen Plus. Again, a good agreement between calculated and reported values is observed, generally less than 2% except for water vapor and nitrogen which has error of around 5%.

**Table 2.** Chemical composition of each state for Booster Compression as calculated by Aspen Plus and the relative error when compared with reported values from heat and mass flow diagram.

Component	Aspen Plus							Relative error (%)						
	8	8(A)	9(A)	10(A)	11(A)	12(A)	13(A)	8	8(A)	9(A)	10(A)	11(A)	12(A)	13(A)
Carbon dioxide	0.45	0.45	0.45	0.45	0.45	0.45	0.01	0.07	0.07	0.07	0.07	0.07	0.07	1.02
Water	0.00	0.00	0.00	0.00	0.00	0.00	0.99	5.06	5.06	5.06	5.06	5.06	4.36	0.01
Nitrogen	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.28	0.28	0.28	0.28	0.28	0.28	5.87
Methane	0.45	0.45	0.45	0.45	0.45	0.45		0.24	0.24	0.24	0.24	0.24	0.24	
Ethane	0.05	0.05	0.05	0.05	0.05	0.05		0.08	0.08	0.08	0.08	0.08	0.08	
Propane	0.03	0.03	0.03	0.03	0.03	0.03		0.24	0.24	0.24	0.24	0.24	0.24	
Isobutane	0.01	0.01	0.01	0.01	0.01	0.01		0.65	0.65	0.65	0.65	0.65	0.65	
N-butane	0.01	0.01	0.01	0.01	0.01	0.01		0.87	0.87	0.87	0.87	0.87	0.88	

Table 3 shows the calculated results for the chemical composition of each state in Sales Gas Compression and the relative error between the calculated from DWSIM and reported values from heat and mass flow diagram. Again, they show an excellent agreement between calculated and reported values. For this process, the isobutane is the component that has highest relative error at around 2%.

**Table 3.** Chemical composition of each state for Sales Gas Compression as calculated by DWSIM and the relative error when compared with reported values from heat and mass flow diagram.

Component	DWSIM						Relative error (%)					
	20	21	22	23	24	25	20	21	22	23	24	25
Carbon dioxide	0.22	0.22	0.22	0.22	0.22	0.22	0.18	0.18	0.18	0.18	0.18	0.18
Nitrogen	0.01	0.01	0.01	0.01	0.01	0.01	0.26	0.26	0.26	0.26	0.26	0.26
Methane	0.64	0.64	0.64	0.64	0.64	0.64	0.18	0.18	0.18	0.18	0.18	0.18
Ethane	0.07	0.07	0.07	0.07	0.07	0.07	0.18	0.18	0.18	0.18	0.18	0.18
Propane	0.04	0.04	0.04	0.04	0.04	0.04	0.74	0.74	0.74	0.74	0.74	0.74
Isobutane	0.01	0.01	0.01	0.01	0.01	0.01	1.98	1.98	1.98	1.98	1.98	1.98
N-butane	0.01	0.01	0.01	0.01	0.01	0.01	1.46	1.46	1.46	1.46	1.46	1.46

For the chemical composition as calculated by Aspen Plus for the Sales Gas Compression, the relative error is smaller than 0.0001%. In other word, the calculated and reported values are almost the same, thus the table reporting these values are not included here for brevity.

## 5. Conclusion

The chemical processes related to offshore petroleum production facilities, namely, Booster Compression and Sales Gas Compression, were used as examples to demonstrate of the capabilities of both Aspen Plus and DWSIM. Based on four important parameters presented, it appeared that these two codes could model the gas compression processes and produced consistent simulation results between each other and in good agreement with real plant data. For the same process and equipment, the discrepancy between simulation results of DWSIM and Aspen Plus was less than 5% except for certain nodes. It has been demonstrated that free and open-source software like DWSIM could potentially perform similar tasks as commercial software, Aspen Plus. It was found that DWSIM was able to simulate chemical processes and calculate the thermodynamic properties and chemical composition quite accurately especially for the gas products. The relative errors for chemical composition and absolute errors for state properties were mostly found to be within 5% which is considered acceptable. The results showed that the simulation accuracy from DWSIM is similar to Aspen Plus. In conclusion, DWSIM could serve as an alternative process modeling software especially for offshore petroleum production.

## Acknowledgment

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