UMUTEME, O.M., ISLAM, S.Z., HOSSAIN, M. and KARNIK, A. 2023. Modelling hydrate deposition in gas-dominant subsea pipelines in operating and shutdown scenarios. *Sustainability* [online], 15(18), article number 13824. Available from: <u>https://doi.org/10.3390/su151813824</u>

Modelling hydrate deposition in gas-dominant subsea pipelines in operating and shutdown scenarios.

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2023



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Article Modelling Hydrate Deposition in Gas-Dominant Subsea Pipelines in Operating and Shutdown Scenarios

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Abstract: This study addresses a significant research gap related to hydrate formation in subsea gas pipelines, with a specific focus on deposition rates during shutdown scenarios, which has received limited attention in previous studies. Past research has employed various methodologies, including experimental, analytical, and computational fluid dynamics (CFD) approaches, to predict hydrate formation conditions, but none have tackled the prediction of hydrate deposition during shutdowns. In this study, we employ a multiple linear regression modeling approach using the MATLAB regression learner app. Four distinct regression models were developed using data generated from 81 CFD simulations, utilising a 10 m length by 0.0204 m diameter 3D horizontal pipe model in Ansys Fluent, as previously developed Through cross-validation against experimental data, the standard linear regression model emerged as the most reliable choice for predicting hydrate deposition rates, providing predictions within $\pm 10\%$ uncertainty bounds of experimental results up to pressures of 8.8 MPa at hydrate-forming temperatures. The uniqueness of this new model lies in its ability to estimate the risk of hydrate deposition in subsea gas pipelines, especially with low gas flow rates and during shutdown periods, which are critical for maintenance planning. Furthermore, by estimating depositional volumes, the model predicts hydrate slurry volumes at receiving facilities, contributing to energy sustainability and benefiting gas transport pipeline operators, particularly in aging gas fields with declining production.

Keywords: hydrate deposition rate; linear regression modelling; subcooling temperature; gas pipeline; pipeline diameter

1. Introduction

The importance of addressing gas hydrates in pipelines for both energy sustainability and industry applicability remains a continuous research concern. This reflects the ongoing efforts and focus within the energy industry and the scientific community to find solutions and develop strategies for managing gas hydrates to ensure the efficient and sustainable transportation of energy resources. Efforts to develop predictive models and favour cleaner energy sources such as natural gas contribute to achieving more sustainable energy practices within the oil and gas sector. The formation of hydrates in subsea gas-dominant pipelines continues to obstruct the safe flow of gas to processing plants. Hydrate deposition occurs very fast within the first hour of hydrate formation, and can plug the pipeline more quickly when large mass of hydrates are detached from the wall by sloughing events [1]. Therefore, estimating the deposition rate of hydrates allow for the estimation of the volume of hydrates deposited and the severity of hydrate plugging events within a given period of pipeline operation. The emphasis on predicting hydrate deposition rates has been studied using experiments [2–4], analytical models [5,6], and CFD models [7,8]. The experiments have provided the basis for understanding the flow parameters influencing the deposition rates of hydrates in gas pipelines through parametric analysis of the effect of subcooling temperature, water volume fraction, gas velocity, and pipeline diameter. Therefore, it is



Citation: Umuteme, O.M.; Islam, S.Z.; Hossain, M.; Karnik, A. Modelling Hydrate Deposition in Gas-Dominant Subsea Pipelines in Operating and Shutdown Scenarios. *Sustainability* **2023**, *15*, 13824. https:// doi.org/10.3390/su151813824

Academic Editors: Mohammad Reza Pendar and Frederico Miguel Freire Rodrigues

Received: 16 August 2023 Revised: 4 September 2023 Accepted: 9 September 2023 Published: 16 September 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). possible to formulate a multiple linear regression model where hydrate deposition rate is the dependent variable. Previous studies adopted machine learning regression modelling of hydrate formation equilibrium temperature and pressure [9–14]. The multiple regression approaches implemented in the cited literature include the use of genetic algorithm (GA), least square support vector machine (LSSVM), and support vector machine (SVM). Recently, hydrate volume fraction was predicted using regression modelling [15]. Again, Yu and Tian (2022) [16] adopted random forest, naive Bayes, and support vector regression to determine hydrate formation conditions for pure and mixed hydrate-forming gases. However, no regression modelling approach has been adopted to specifically predict the deposition rate of hydrates in gas pipelines. The results of the improved hydrate deposition rate CFD model in our previous publication [7] compared more favourably with experimental data in relation to existing models [6,17], especially at low gas velocities. Hence, the CFD model has been adopted in simulations for this study. Also, in contrast to current machine learning models that focus solely on predicting the conditions for hydrate formation, the CFD model goes a step further by predicting hydrate depositional rates. This improvement aims to enhance routine maintenance planning for gas pipelines prone to hydrate formation. Estimating the depositional volume in L/min, as recommended in previous experimental studies [2,4], enables us to approximate the volume of hydrate slurries expected at the receiving facility. This study's specific contribution to knowledge lies in quantifying and estimating the risk of hydrate deposition in gas pipelines, particularly with lower gas flow rates and during shutdown scenarios. Aging gas fields experiencing declining production encounter low gas flow rates, which significantly impact routine maintenance planning. By utilising our model to estimate the severity of hydrate formation during shutdown scenarios, gas transport pipeline operators in the oil and gas industry can benefit from improved decision-making and enhanced flow assurance.

Regression modelling is implemented when the data to be observed are not easily accessible and measured from the field, and this is applicable to measuring the deposition rate of hydrates in industry-scale gas pipelines. The following necessary conditions for the formation of natural gas hydrates are stated in the literature [18] as follows: firstly, a specific combination of low temperature and high pressure must be present, determined by the composition of the gas. Secondly, gas hydrate formers such as methane, ethane, and carbon dioxide need to be present. Thirdly, an adequate amount of water is required. Additionally, the literature suggests that two other factors equally contribute to hydrate formation: turbulence resulting from high flow velocity and agitation, and the presence of nucleation sites such as elbows, tees, and valves, as well as free water, which facilitates a favourable water-gas interface for nucleation. However, based on the parametric studies conducted in the literature [3,4,6], this study proposes a regression model with subcooling temperature (ΔT), pipeline diameter (D), water volume fraction (α_w), and gas velocity (V) as predictors, while the deposition rate of hydrates (Q_{hd}) is the dependent variable. This is to further ensure that the prediction of hydrate deposition rate is handy in the field, so that the model can be used as a quick predictor of the risk of pipeline plugging by hydrates. The prediction of hydrate deposition rates at lower gas velocity of 4.7 m/s by the CFD model developed in our previous paper [7] were more representative of experimental predictions than the existing analytical model by [6]. Hence, the data used in developing the multiple regression model have been simulated from the validated CFD model for predicting the deposition rate of hydrates. Another driver for this study is the need to predict the deposition rates of hydrates when the pipeline is shut down if depressurisation is not affected. The deposition of hydrates has been reported in gas pipelines during shutdown due to unforeseen operational problems without the need to depressurise the line [19–22]. However, it is not possible to simulate this condition using CFD by setting the gas flow velocity as "zero". Hence, with a multivariate regression model, the deposition rate can still be predicted by setting the velocity term to zero. Usually, cooldown times are up to 24 h [21] or 48 h [19], and it is important to estimate the amount of hydrates deposited within this shutdown period. Multiple regression modelling is implemented to identify the best combination of the predicting variables [23] when the independent variables are more

than one [24]. In this study, the combination of the predictor variables has been selected based on the parametric sensitivity simulations conducted in our previous paper [7] and the effects of subcooling temperature and gas velocity on the empirical deposition of rates of hydrates [3,4].

2. Method

This study develops an approximating function for the deposition rate of hydrates in gas-dominant subsea pipelines, operating in environmental temperature conditions that favour hydrate formation. The main assumption in this study is that the rate of hydrate deposition in a pipeline can be accurately predicted by the gas velocity, water volume fraction, subcooling temperatures, and pipeline diameter from empirical evidence [2–4,6,7]. Stable hydrates form when the system temperature is below the hydrating equilibrium condition for stable hydrates. The subcooling temperature reduces the gas temperature by the subcooling value into the stable hydrates zone. The equilibrium pressure must be lower than the operating pressure of 8.0 MPa and the pipeline temperature must be less than 292 K to ensure that hydrates are forming before using this regression model. The equilibrium hydrate formation pressure equation for methane temperature ranging from 0-25 °C by Sloan and Koh (2007) [25] is adopted to compute the minimum pressure required for hydrate formation. Stable hydrates are formed at temperatures below 292 K for methane hydrates as discussed in the literature [2,7]. Hence, the regression model is for natural gas with methane gas above 82% by composition. The model is based on the parametric simulations conducted using the validated CFD model for predicting the deposition rates of hydrates mentioned earlier. The data are made up of 81×5 matrix data table with a total of 405 data. The basis for the selected variables is discussed as follows based on evidence in the literature [2-4,6,7]: (i) gas velocity defines the nature of fluid flow—laminar, transitional, or turbulent; (ii) hydrate formation, agglomeration, and pipe wall deposition are affected by the gas velocity; (iii) increase in gas velocity under the same pressure and subcooling temperature increases the deposition rates of hydrates; and (iv) increasing the subcooling temperature of the pipeline at constant gas velocity also increases the deposition rate of hydrates. Also, the additional outcome of the CFD simulations proposes that: (i) an increase in pipeline diameter under the same gas flow condition increases the deposition rate by similar factor; and (ii) an increase in the volume fraction of water reduces the deposition rate of hydrates. The developed regression model was validated with experimental studies. The stages of the adopted method In the development, validation, and application of this regression model are presented in Figure 1 below.



Figure 1. Methodology.

2.1. Defining Variables and Data Generation

The data for the regression model development were obtained from the CFD simulations. The measured variables are defined based on the parametric studies conducted in the literature [7]. The validated CFD model is a 10 m length by 0.0204 m diameter pipe and a wall thickness of 0.0012 m. Given that the pipeline is constructed from steel, in order to mitigate the impact of pipe wall thickness on subcooling temperature, the entire wall was adjusted to match the hydrate-forming temperature. Initial multiphase flow is made up of natural gas and water. The simulation was conducted in a commercial CFD software-ANSYS Fluent, version 2020 R1. The architecture of the computer for the simulations is designed with Intel Xeon Gold 6230 quad-core 2.10 GHz CPU and RAM of 16 GB. Input variables are operating pressure, temperature, water volume fraction, and gas velocity. This research utilises the Eulerian–Eulerian multiphase framework, incorporating boundary conditions and physical flow parameters primarily to improve the interaction between gas and water interfaces. Previous computational fluid dynamics (CFD) simulations focusing on gas hydrates have favoured the Eulerian–Eulerian approach as the most suitable method for enhancing interfacial interactions between gas and water [26,27]. Since hydrate deposition on the pipe wall is a near-wall viscous effect, the realisable $k-\varepsilon$ two-equation turbulence model was employed to improve the modeling of near-wall viscosity in predicting the deposition of hydrates [7,28]. In order to improve the efficiency of multiphase flow in the oil and gas sector, pipeline designs aim to minimise frictional losses and pipe wall erosion, thus reducing pressure drops. Consequently, the study enhanced the stability of the computational fluid dynamics (CFD) simulation by selecting a mesh size that yielded the least noticeable pressure drop, as determined through a sensitivity analysis of the mesh grid. This mesh sensitivity analysis was conducted at specific conditions: an inlet velocity of 10 m/s (equivalent to a flow rate of 3.3 kg/s), a temperature of 292 K, and a pressure of 8.8 MPa. The simulation was conducted for different ranges of pipe diameter, gas velocity, subcooling temperatures, and water volume fraction. A total of eighty-one (81) deposition rates of hydrates were predicted from 81 simulations. The sample size was determined as per the recommendation in the literature [29,30] using G*Power software, version 3.1 [31], with a conservative effect size of 0.30 because the CFD model was already validated with experimental results, and statistical power of 95%, which yielded a minimum sample size of 72. Detail documentation on the development and validation of the CFD model is already discussed in the literature [7,32]. The input variables for the CFD simulations are defined in Table 1 as follows.

Table 1. Range of input data for CFD simulations.

Variables	Range
Gas Velocity (m/s)	2.0-8.8
Subcooling Temperature (K)	1.0–9.0
Water Volume Fraction (-)	0.02-0.12
Pipe diameter (m)	0.0204-0.0612
Hydrate Deposition Rate (L/min)	0.0370-0.7030

2.2. Regression Model Development

The regressor variables are as defined earlier, including the subcooling temperature (ΔT), pipeline diameter (D), water volume fraction (α_w), and gas velocity (V) as predictors, while the deposition rate of hydrates (\dot{Q}_{hd}) is the outcome variable. This is represented in Figure 2, below.



Figure 2. Interaction of regressor variables with the deposition rate of hydrates.

Selecting a multiple regression model with the most appropriate explanatory and predictive power is difficult and depends on the selection of an appropriate set of variables that defines the expected response. In MATLAB, multiple regression modelling can be achieved by the standard linear regression, robust linear regression, interaction linear regression, and stepwise linear regression. The standard linear model is also known as ordinary least square (OLS) estimation of the intercept and coefficients to minimise the error sum of the squares [29]. However, there are instances where the data sets contain values that have high discrepancy from the expected outcome, also known as outliers. When this occurs, as with some experimental outcomes, an alternative approach using robust linear regression may be adopted. The robust linear regression modelling approach produces improved estimates by minimising the weights given to outlying cases when calculating the regression coefficients [29]. Thus, the presence of outliers in the data sets is ruled out when the outcome of the robust linear regression model compares favourably with the predictions of the OLS model. Both models are represented in Equation (10). The stepwise linear regression modelling approach in Equation (11) was considered to enhance the predictability of hydrate deposition rates in MATLAB. In the stepwise regression approach, one variable at each stage is selected from a group of predictors that produces the highest coefficient of determination (R^2). The selected variable is the regressor that produces the largest value of F statistic [24], implying that variables are either added or removed at each step leading to an iterative sequence of regression modelling. However, one problem with this approach is the high dependence on chance and the likely underestimation of predictive confidence intervals [29]. In the equation, two sets of interactions between two regressors were included with the four additive regressors in the OLS equation (Equation (10)). The last approach adopted is the interaction linear regression model in Equation (12). In the interactions approach, additional sets of interacting variables are added to the additive models of the original regressors as in the OLS. Here the interaction predictors are products of the original predictors [29]. The regression modelling approach adopted in this study did not consider a squared form of input variables to prevent over-fitting, where the model fits the training data too closely. Again, when squared terms are introduced into linear regression models, the assumption of a linear relationship between the predictor variables and the response variable can be undermined and the model becomes nonlinear. Furthermore, our adoption of a linear modelling approach is supported by the experimental results in the literature [2,4] used for the model validation.

2.3. Model Selection Criteria

The adopted model for the parametric studies was based on a combination of five model selection criteria, including the error sum of squares (SS_E), adjusted R-squared (R^2adj .), Akaike information criterion (*AICc*), standard F test, and root of mean square error (*RMSE*). Statistical significance was determined using the *p*-value at alpha (α) level

of 0.05. Lowering the significance level below 0.05 may shift the focus towards statistical significance at the expense of practical significance in the study, primarily due to the model's limited ability to detect lower deposition rates. This shift can reduce proactive predictability and increase the vulnerability of the pipeline to hydrate plugging events. Each criterion is discussed further to provide insight into the parameters that influenced the predictive power of the chosen model.

Error sum of squares (SS_E): In regression analysis, the sum of squares is used to explain the dispersion of the data sets around a mean. The residual sum of squares, or error sum of squares as used in this study, is based on the residual after the model-fitting process. SS_R represent the regression sum of squares of the data set that predicted the model-fit regression line. The total sum of squares (SS_T) describes the total variability in the research data. The estimation of SS_E , SS_R , and SS_T are defined in Equations (1)–(3) below.

$$SS_E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
(1)

$$SS_R = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$$
 (2)

$$SS_T = SS_R + SS_E = \sum_{i=1}^n (y_i - \overline{y})^2$$
(3)

where SS_R is the regression sum of squares; \hat{y}_i , is the predicted value per data point; y_i , is the original target value; \bar{y} is the mean of the data set representing the regression line prediction, and $y_i - \bar{y}$, is the deviation of the predicted value per data from the mean.

Adjusted R-squared (R^2adj .): The coefficient of determination (R^2) is determined from the ratio of the SS_E and SS_T (Equation (4)). Since it is a ratio where the denominator is always higher or equal to the numerator, the value is from 0 to 1. The value of R^2 indicates the extent to which the variance in the predicted variable is dependent on the predictor variables. However, because the value of R^2 increases as new variables are added to the regression equation, it is seldom problematic in determining model fit when comparing models. To overcome this weakness, the R-squared is adjusted (R^2adj .) as in Equation (5) to compensate for this effect, so that the R^2 value decreases as more predictor variables are added to the regression model [24], hence guarding against overfitting. Consequently, it is important to select the predictors that have a higher effect on the variance of the response variable.

$$R^2 = \frac{SS_E}{SS_T} \tag{4}$$

$$R^{2}adj. = 1 - \left(1 - R^{2}\right)\frac{n - 1}{(n - k - 1)}$$
(5)

where n - k - 1 is the degree of freedom for the denominator, *k* represents the numbers of the measured predictor variables, and *n*, the total data points.

Standard F test: Another statistical measure for model selection is the standard F test, which tests the significance of the obtained value of the R^2 . It is used to determine if the set of predictor variables statistically explain a significant amount of the outcome. Higher values of F indicate better model performance. F test is estimated from Equation (6).

$$F = \frac{R^2(n-k-1)}{k(1-R^2)}$$
(6)

where *k* represents the numbers of predictor variables and n - k - 1, the statistical degree of freedom. Similarly, the *p*-value measures the statistical significance of the regression model or individual coefficients within the model and assesses the probability of obtaining the observed regression coefficients. The *p*-value is not directly used in model selection;

however, it does provide evidence of the strength of the contributing variables in regression analysis.

Root of mean square error (*RMSE*): This model selection measure is the standard deviation of the prediction errors or residuals. The *RMSE* provides insight into how far the error is from the prediction. Models with lower *RMSE* have higher predictive power. The *RMSE* is estimated from Equation (7) below, where the symbols n, \hat{y} , and y_i are as defined earlier.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2}$$
(7)

Akaike information criterion (*AICc*): The *AICc* enhances the selection of the most fit-for-purpose model because it compares the quality of each model against the other models. It measures the estimated prediction error and the relative quality of a set of data. The smaller case "c" in Equation (9) indicates that the calculated *AIC* value has been corrected for smaller samples to prevent overfitting because of the inclusion of both stepwise and interaction models in this study. The *AIC* criteria is generally an estimation of the information loss because of the presence of the likelihood function, \hat{L} . This index also take into account the number of regression coefficients being tested [29]. When the experimental data sets for cross-validation are sparse, the *AICc* have been found to be more reliable than the F test [33]. The smaller the value of *AICc*, the better the model fit. *AIC* is estimated using Equation (8).

$$AIC = 2k - 2In(\hat{L}) \tag{8}$$

$$AICc = AIC + \frac{2k^2 + 2k}{n - k - 1} \tag{9}$$

where \hat{L} is the likelihood function, k is the numbers of predictor variables, and n - k - 1, the statistical degree of freedom, implying that the higher the variables, the higher the *AIC* value. Thus, from the discussion above, the model selection criteria are defined as follows (Table 2).

Table 2. Criteria for model selection.

Parameter	Criteria
R^2 adj.	Higher
SS_E	Lower
RMSE	Lower
AIC_{c}	Lower
F-Test	Higher

A simple ranking method was adopted, where the most favourable of the four models was awarded a score of 4 and the least favourable model was awarded a score of 1 on each selection parameter. The model with the highest sum was adopted for the prediction of hydrate deposition rates.

3. Result, Validation, Model Selection, and Discussion

3.1. Results

The data retrieved from the CFD simulation were trained in the regression learner application in MATLAB version R2020a and the coefficient for each predictor variable was recorded as presented in Table 3, for each regression model investigated. The *p*-value for each coefficient is also indicated as defined below (Table 3).

Parameter Estimates	Standard Linear Regression	Robust Linear Regression	Stepwise Linear Regression	Interaction Linear Regression
β_0	-0.0845 *	-0.0615	-0.4770 ***	-0.0129
β_V	0.0163 ***	0.0131 ***	0.0156 ***	-0.0105
$\beta_{\Delta T}$	0.0252 ***	0.0240 ***	0.0531 ***	-0.0268
$\beta \alpha_w$	-3.4127 ***	-3.3872 ***	2.5804	2.2833
β_D	7.3412 ***	7.5444 ***	12.3156 ***	7.0976 ***
$\beta_{\Delta T}$, $\beta \alpha_w$	-	-	-0.4020 *	-0.0372
$\beta \alpha_{w.} \beta_D$	-	-	-77.0638 ***	-80.6991 ***
$\beta_{V}, \beta_{\Delta T}$	-	-	-	0.0049
$\beta_{V.}\beta\alpha_{w}$	-	-	-	-0.2666
β_V, β_D	-	-	-	0.2793
$\beta_{\Delta T.} \beta_D$	-	-	-	0.5397 *

Table 3. Coefficients of predictor variables for each regression model.

p < 0.1; p < 0.05; p < 0.05; p < 0.01.

At alpha (α) level of 0.05, all the predictor variables have coefficients with a high level of significance for the standard linear and robust linear regression models. For the stepwise linear regression model, the coefficient for the water volume fraction is not statistically significant. For the interaction linear regression model, only the coefficients for pipeline diameter and the interaction between water volume fraction and pipeline diameter are statistically significant. The corresponding regression equations based on the coefficients in Table 3 are of the forms stated in Equations (10)–(12) below. All coefficients are standardised.

Standard and robust linear regression

$$Q_{hd} = \beta_0 + \beta_v V + \beta_{\Delta T} \Delta T + \beta_D D + \beta_{\alpha_w} \alpha_w \tag{10}$$

Stepwise linear regression

$$\dot{Q}_{hd} = \beta_0 + \beta_v V + \beta_{\Delta T} \Delta T + \beta_D D + \beta_{\alpha_w} \alpha_w + \beta_{\Delta T} \beta_{\alpha_w} \Delta T \alpha_w + \beta_{\alpha_w} \beta_D D \alpha_w$$
(11)

Interaction linear regression

$$Q_{hd} = \beta_0 + \beta_v V + \beta_{\Delta T} \Delta T + \beta_D D + \beta_{\alpha_w} \alpha_w + \beta_{\Delta T} \beta_{\alpha_w} \Delta T \alpha_w + \beta_{\alpha_w} \beta_D D \alpha_w$$

$$+ \beta_v \beta_{\Delta T} V T + \beta_v \beta_{\alpha_w} V \alpha_w + \beta_v \beta_D V D + \beta_{\Delta T} \beta_D T D$$
(12)

where β_0 is the intercept of the model and β_v , $\beta_{\Delta T}$, β_D , and β_{α_w} are the partial regression coefficients of the respective regressor variables—gas velocity (V, m/s), subcooling temperature (ΔT , K), pipe diameter (D, m), and water volume fraction (α_w , dimensionless), as defined earlier. The regression graphs in Figure 3 are the outcome of each model predictions compared with the original CFD hydrate deposition rates. As seen from the regression graphs, the R-squared values for interaction linear regression model and the stepwise linear regression model can have the error of overfitting because of the increase in predictor variables.

The R^2 value of 0.867 for the interaction model in Figure 3 outperforms other models. However, the rejection of the interaction model is based on the use of a combination of model selection criteria presented in Table 2 and the performance when compared with experimental data as discussed further in subsequent sections. Absence of outliers is confirmed from the standard and robust regression models as the calculated R-squared have approximately similar values of 0.8170 and 0.8134, respectively. In Figure 4, the residual plots indicate that the residuals reduce as the hydrate deposition rate increases for both the standard linear and robust linear regression models. The residuals for the interaction linear and stepwise linear regression models are spread across the deposition rates when compared to the standard linear and robust linear solution rate increases for both standard linear and reduction in prediction error as the deposition rate increases for both standard linear and the robust linear models suggests that the predictor coefficients can account for a higher variance in the deposition rate when the pipeline is most vulnerable, implying further that both models are highly suitable in capturing higher risks of hydrate plugging events from deposited hydrates. The most suitable model will be selected after validation with experimental results.



Figure 3. Comparing plots for each regression modelling approach.



Figure 4. Residuals plots for each regression modelling approach.

3.2. Validation of Models with Experimental Data

In Table 4, the predictive power of each model was validated with experimental data at lower and higher gas velocities. Most importantly, the sensitivity of the regression models to changes in subcooling temperatures at a lower velocity of 4.6 m/s were within $\pm 10\%$ of experimental outcomes, compared to the predictions of the analytical model in Di Lorenzo et al. (2018) [6].

Table 4. Validation of regression models with experimental of
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	Inp	ut Data		Experimental	CFD Model Hydrates	Predicted H	ydrates Deposition R	ate (L/min) by Regre	ssion Models	
Gas Velocity —V(m/s)	Subcooling Temperature— ΔT(K)	Water Volume Fraction— α_W (-)	Pipe Diameter —D(m)	Hydrates Deposition Rates (L/min)	Deposition Rates (L/min)—Umuteme et al., (2022) [7]	Standard Linear Model	Robust Linear Model	Interaction Linear Model	Stepwise Linear Model	Experiment References
4.6 4.6 4.6	4.5 6.0 7.5	0.06 0.06 0.06	0.0204 0.0204 0.0204	0.06 0.08 0.11	0.06 0.10 0.13	0.05 0.09 0.12	0.06 0.09 0.13	0.09 0.10 0.11	0.04 0.08 0.12	Aman et al. (2016) [4]
8.8 8.8 8.8 8.8 8.8	2.5 4.3 7.1 8.0	0.06 0.06 0.06 0.06	0.0204 0.0204 0.0204 0.0204	0.07 0.13 0.15 0.19	0.06 0.13 0.14 0.18	0.07 0.11 0.18 0.21	0.06 0.11 0.17 0.20	0.05 0.10 0.17 0.19	0.04 0.10 0.18 0.20	Di Lorenzo et al. (2014) [3]

In Figure 5, the outcome of the predictive regression models was compared and the R^2 value of the standard linear model was the highest. However, the closeness of the R^2 value for the standard linear model to the R^2 values for the other regression models suggests that the R^2 is not independently suitable to defend the choice of the final selected model. This is because the predictor variables in all the models were able to account for more than 80% variance in the deposition rates of hydrates. The predictions' goodness of fit is in the following ascending order: interaction linear regression (0.01349) > standard linear regression (0.01336) > stepwise regression (0.01078) > robust linear regression (0.006881). However, only two coefficients of the equation for the interaction linear model were

significant at p < 0.05. Hence, the most appropriate model is the standard linear regression model with the highest goodness of fit value of 0.01336. The final model will be selected after considering other criteria discussed in Table 2.



Figure 5. Prediction of experimental results by each regression modelling approach.

A further investigation of the predictive power of the regression models along the experimental data sets suggest close predictions by all models at lower and higher deposition rates of hydrates (Figure 6). However, as the experimental deposition rate increased to 0.24 L/min, only the standard linear model was able to indicate the capability of higher out-of-data predictive power. The assumption of homoscedasticity and normality must be fulfilled in linear regression modelling, else a non-linear approach is adopted [29]. The test for normality and the consistency of the prediction of the models by fulfilling homoscedasticity was investigated using the normal probability plot (Q–Q plot) in Figure 7. The Q–Q plot normality test suggests that the predicted results are from the same population if the plot resembles a straight line [23], The linear nature of all the predicted results also aligns with experimental outcome, indicating the ability of the models to predict hydrate deposition rates beyond the training data from the CFD model. The certainty of accurate predictions as compared with experimental data is observed at 90% confidence interval on the Q–Q plot in Figure 7a, and indicates higher predictive power at higher deposition rates above 0.15 L/min. All the predictions are within a 10% prediction band of the normal probability plot when compared with experimental values as indicated in Figure 7b. The

selection of a 90% confidence interval and a 10% prediction width was made to guarantee that the range encompasses observed experimental values.



Figure 6. Comparing predictions by each regression modelling approach with experimental results.



Figure 7. Normal probability plots. (a) With 90% certainty band. (b) With 10% prediction band.

3.3. Model Selection

The close predictions among the models as discussed in Section 3.2 above show that the data generated using the CFD model are of experimental quality. In this section, the preferred regression model was selected using the criteria discussed in Section 2.3. In Table 5, a comparison of the values for each model fit selection criteria is presented. The model selection criteria are based on a combination of adjusted R-squared, error sum of squares, RMSE, AICc criteria, and F test, as defined earlier (Table 2). In Table 6, the model selection parameters have been ranked in the order that aligns with the criteria for model selection (Table 2), where 4 is given to the regression model that is most representative of the set criteria and 1 for the least representative regression model for each model fitness selection criteria.

Parameter	Standard Linear Regression	Robust Linear Regression	Stepwise Linear Regression	Interaction Linear Regression
R ² adj.	0.9597	0.9204	0.9264	0.8547
SSE	0.0007	0.0011	0.0015	0.0017
RMSE	0.0106	0.0138	0.0156	0.0168
AICc	-50.730	-47.080	-45.300	-44.300
F-Test	5.752	2.817	3.063	1.452

Table 5. Comparing values of each model selection criteria for all regression models.

Table 6. Parameter ranking based on fitness of each regression model to experimental results.

Parameter	Standard Linear Regression	Robust Linear Regression	Stepwise Linear Regression	Interaction Linear Regression
R ² adj.	4	2	3	1
SS_E	4	3	2	1
RMSE	4	3	2	1
AICc	4	3	2	1
F-Test	4	2	3	1
Total Score	20	13	12	5

The standard linear model with the highest sum of model fit score in Table 6 is selected. Again, a comparison of the normalised violin plots in Figure 8, which visualise the distribution of numerical data, indicates that the shape of the standard linear model is a close match to the experimental data. Also, from Table 3, only the coefficients of the standard linear model exhibit statistical significance at an alpha level of 0.05.



Figure 8. Normalised violin plots.

Therefore, the representative equation for the standard linear model based on the coefficients in Table 3 are presented below.

$$Q_{hd} = 0.0163V + 0.0252\Delta T - 3.4127\alpha_w + 7.3412D - 0.0845$$
(13)

In Table 3, the *p*-value of the measured variables (pipe diameter, gas velocity, subcooling temperatures, and water volume fraction) for the standard linear model are <0.01, suggesting stricter predictability. The relative impact of each predictor variable on hydrate deposition rate can be inferred from Equation (13), as presented in Table 7.

Predictor Variable	Sensitivity (other Variables Held Constant)	Impact on Hydrates Deposition Rate
Gas Velocity	Increase Decrease	Increase Decrease
Subcooling Temperature	Increase Decrease	Increase Decrease
Pipeline Diameter	Increase Decrease	Increase Decrease
Water Volume Fraction	Increase Decrease	Decrease Increase

 Table 7. Relative impact of each predictor variable on hydrate deposition rate.

As indicated in Table 7, velocity, subcooling temperature, and diameter have increasing effect, while water volume fraction has a reducing effect on the deposition rate of hydrates. Hence, increasing the velocity while keeping other variables constant will increase the deposition rate of hydrates. Again, at constant velocity, increasing the subcooling temperature increases the deposition rate of hydrates. Similarly, keeping other variables constant, the deposition rates of hydrates increase with an increase in pipeline diameter. This is due to the increase in the volume of gas [7]. Finally, as other variables are constant, increasing the water volume fraction enhances transportability while reducing deposition rate. Again, the gas velocity, volume fraction of water, and the pipe annulus approaches zero as the hydrate deposition rate increases. Consequently, the stability of hydrates in the pipe becomes solely dependent on the subcooling temperature, implying that increasing the temperature of the pipeline can reduce the thickness of deposited hydrates in a gas pipeline. Another important feature of this model is being able to predict the deposition of hydrates when the velocity is set to "0", as applicable during pipeline shutdown scenario. Thus, this regression model satisfies the theoretical position on hydrate deposition and transportability in subsea gas pipelines (e.g., Aman et al., 2016; Berrouk et al., 2020; Sule et al., 2015 [4,27,34]). As indicated earlier, the practical application of the regression model developed in this study is premised on the assumption that the gas temperature is below the hydrate equilibrium temperature of 292 K for natural gas with predominantly methane compositional value above 80%. The operating pressure for the CFD model was set at 8.8 MPa for all simulations. Lower pressures predicts lower deposition rates [19]. Hence, the prediction of this model is proactive and represents the worst-case scenario at operating pressure less or equal to 8.8 MPa.

3.4. Discussion

The study evaluated multiple regression models, including standard linear, robust linear, stepwise linear, and interaction linear regression models, to predict hydrate depositional rates in gas pipelines. The study identified key predictor variables affecting hydrate deposition rates in gas pipelines including velocity, subcooling temperature, diameter, and water volume fraction. These variables have been simulated with a validated CFD model in the literature [7]. Model selection criteria, including adjusted *R*-squared, error sum of squares, *RMSE*, *AICc*, and F test, were used to select the most suitable regression model. The results show that all models, including the standard linear model, are capable of accurately predicting hydrate deposition rates, even beyond the training data. The analysis further reveals that the standard linear model consistently outperforms other models based on the selection criteria. Among these models, the standard linear model with the highest sum of model fit score was adopted. The standard linear model has an impressive R-squared value of 0.9597, indicating a strong ability to explain the variance in hydrate deposition rates. To

assess the reliability of the regression models, validation was conducted using experimental data, especially at both lower and higher gas velocities. The closeness of the standard linear model predictions to experimental outcomes highlights the models' accuracy. In particular, the regression models demonstrate a high degree of sensitivity to changes in subcooling temperatures at a lower gas velocity. Again, the selected standard linear model indicates that increasing velocity, subcooling temperature, and diameter have a positive effect on hydrate deposition rates, while increasing the water volume fraction reduces deposition rates. Most importantly, the model can predict hydrate deposition even during pipeline shutdown scenarios, thus, providing the necessary flow assurance information during the planned start-up of hydrate-forming gas pipelines.

4. Practical Application of Regression Model

The parametric analysis in this section was performed to investigate the practical application of the selected regression model. These analyses include: (i) the prediction of the deposition rates of hydrates in pipeline shutdown scenarios, (ii) predicting the influence of change in environmental temperature on the deposition rate of hydrates, when the integrity of the pipeline coating and heating system is questionable, (iii) predicting the effect of change in gas velocity based on change in actual gas production, especially at low flow velocity and constant subcooling temperatures, (iv) the influence of pipeline size on hydrate deposition rate during pipeline sizing in design phase, and (v) the influence of water volume fraction on the deposition rate of hydrates.

4.1. Pipeline Shutdown Planning

Estimating the deposition rate of hydrates at zero gas velocity can assist in determining how long a gas pipeline that is experiencing hydrate formation should be shut down. The change in the deposition rate of hydrates was predicted by the model in Figure 9 at the subcooling temperature of 7.0 K, water volume fraction of 0.06, and pipeline diameter of 8 inches (0.204 m).



Figure 9. Change in the deposition rate of hydrates as the gas velocity increases at constant subcooling temperature of 7.0 K, water volume fraction of 0.06, and pipeline size of 8 inches (0.204 m).

An increase in velocity while keeping the subcooling temperature constant increases the hydrate deposition rate. From Figure 9, at the subcooling temperature of 7.0 K and "zero" gas flow velocity, which is the scenario when the line is shut down, the gas pipeline still experiences hydrate deposition at the rate of 1.385 L/min. Hence, the deposition of hydrates is expected if the line is shut down at the pressure and temperature conditions that encourage hydrate formation. This model provides a means to study hydrate deposition when the pipeline is shut down due to process failure or for other maintenance within the gas plant or maintenance of subsea production facilities. Depressurising the pipeline outside the hydrate formation temperature and pressure zone is advised in this instance. However, if it is impossible to keep hydrates out of the line, the total deposition can be estimated by multiplying the deposition rate with the duration that the line was shut down to estimate the expected hydrate deposits in the line. The total expected volume of hydrates is the sum of the deposited and dispersed hydrates. From the indication in the literature [3,5], about 33.3% of hydrates formed are deposited in the wall. Hence, an approximate total expected hydrate in the pipeline can be obtained by multiplying the deposition rate estimated by this model under a shutdown scenario by a factor of 3. The predicted deposition rate of hydrates by the model can be a guide for pigging or chemical injection. Evidence in the literature suggests that the growth of hydrates during shutdown is relatively slow [19,21], leading to lower deposition rates as observed in the model prediction in Figure 9.

4.2. Effect of Change in Subcooling Temperature on Hydrate Deposition

This sensitivity is important in determining the cool-down temperature during a shutdown scenario to prevent hydrate formation and deposition. Also, during change in the surrounding subsea temperature, the effect on the deposition of hydrates can be estimated from the model. The velocity was set to 4 m/s, 0.06 water, diameter of 0.204 m, and the subcooling temperature was varied from 3 K to 9 K. From Figure 10, the deposition rate of hydrates increases as the subcooling temperature increases and vice versa, in agreement with experimental results.



Figure 10. Change in the deposition rate of hydrates as the subcooling temperature increases at constant gas velocity of 4 m/s, water volume fraction of 0.06, and pipeline size of 8 inches (0.204 m).

4.3. Effect of Change in Water Volume Fraction on Hydrate Deposition

This sensitivity studies the effect of increasing the volume fraction of water on the deposition rate of hydrates. In theory, the deposition rate of hydrates reduces but hydrate slurry forms instead, which can enhance transportability [7]. At a subcooling temperature of 7.0 K, constant velocity of 4 m/s, and pipeline diameter of 0.204 m, the volume fraction of water was varied from 0.06 to 0.12 to obtain the regression plot in Figure 11.

As expected from theory, as the water volume fraction increase in Figure 11, the deposition rate of hydrates decreases, implying that in gas lines with high water volume fraction, the probability of having hydrate deposits on the wall of the pipeline is minimal. This effect was studied in Berrouk et al. (2020) [27], where the flow of hydrate slurry was enhanced by increasing the water volume fraction. Most importantly, the model developed in this study can provide insight into the maximum water volume fraction to prevent the deposition of hydrates, which would have required much computer simulation effort to estimate using CFD.



Figure 11. Change in the deposition rate of hydrates as the water volume fraction increases at constant gas velocity of 4 m/s, subcooling temperature, and pipeline size of 8 inches (0.204 m).

4.4. Effect of Change in Pipeline Size on Hydrate Deposition in Design Phase

This effect was predicted in Figure 12 at the subcooling temperature of 7.0 K by keeping the gas velocity constant at 4 m/s, and volume fraction of water at 0.06, while the pipeline diameter is in the range of 4 inches (0.102 m) to 16 inches (0.408 m). The change in pipeline diameter increases the deposition rate of hydrates because of the availability of more gas in the pipeline, implying also that if the flowrate is kept constant and the pipe diameter increases, there is a reduction in flowing pressure.



Figure 12. Change in the deposition rate of hydrates as the pipe diameter increases at constant gas velocity of 4 m/s, subcooling temperature, and water volume fraction.

5. Conclusions

Aside from the experimental, analytical, and CFD approaches, previous studies have adopted machine learning regression modelling of the temperature and associated equilibrium pressure condition for hydrate formation. However, there are no regression models that can predict the deposition rate of hydrates in gas pipelines, especially to predict hydrate deposition during a shutdown scenario. This study closed this gap by adopting a multiple linear regression modelling approach using MATLAB regression learner app to train 81 data sets generated by CFD simulation. Four different regression models were developed and the outcome of the cross-validation using experimental data led to the choice of the standard linear regression model, with predictions that compared more favourably with the experimental validation data. Since lower operating pressures leads to lower formation rates [19], the deposition rates of hydrates predicted by this model are proactive and represent the worst-case scenario at the model operating pressure of 8.8 MPa. The uniqueness of our model lies in its ability to predict hydrate depositional rates in a gas pipeline, surpassing existing models [6,17] by achieving higher comparability with experimental data at a low gas velocity. Unlike current machine learning models that solely forecast temperature conditions for hydrate formation, we go a step further by predicting hydrate depositional rates. This advancement aims to enhance the routine maintenance planning of hydrate-forming gas pipelines. By estimating the depositional volume in L/min, as suggested in previous experimental studies [3,4], it becomes possible to estimate the volume of hydrate slurries expected at the receiving facility. The specific contribution of this study to knowledge is the possibility of quantifying and estimating the risk of hydrate deposition in gas pipelines at lower gas flowrate and during shutdown scenarios. Aging gas fields with declining production face low gas flow rates, which impact routine maintenance planning. The use of our model in estimating the severity of hydrate formation during shutdown scenarios benefits gas transport pipeline operators in the oil and gas industry. The study contributes to energy sustainability by offering simulation tools, providing further insights, and quantitative methodologies to manage hydrate-related challenges efficiently, reduce energy losses, ensure system reliability, and optimise energy transport and infrastructure design. The specific contributions of this study to knowledge are as follows:

- (a) Understanding that hydrate deposition rate increases with subcooling temperature is valuable for energy sustainability. This knowledge can help engineers and operators design pipelines and systems that minimise subcooling, reducing the risk of hydrate formation and blockages. This contributes to efficient energy transport and minimises the need for energy-intensive interventions to clear blockages;
- (b) Being able to quantify and estimate the risk of hydrate deposition in gas pipelines during shutdown scenarios is crucial for energy sustainability. It allows operators to plan for and mitigate potential disruptions, ensuring a consistent and reliable energy supply;
- (c) The regression model provides a quicker and less resource-intensive way to predict hydrate deposition rates in field situations. This is beneficial for energy sustainability as it enables early intervention and maintenance to prevent blockages and energy losses in pipelines;
- (d) The fact that the predicted results by the model are within $\pm 10\%$ uncertainty bounds of experimental results up to 8.8 MPa gas pressure at hydrate-forming temperatures ensures the accuracy of hydrate-related predictions. This accuracy is essential for optimising gas transport pipelines, reducing inefficiencies, and minimising resource wastage for planned maintenance;
- (e) Using the model's predicted results as advisory input during pipeline sizing in the design phase helps engineers choose the right pipeline diameter to manage hydrate formation and deposition efficiently. Proper sizing reduces energy losses and ensures sustainable energy transport;
- (f) The model's ability to determine the water volume fraction that aids hydrate transport is essential for energy sustainability. It assists in designing pipeline systems that can safely transport hydrates while minimising the risk of blockages;
- (g) The model's capability to estimate the expected volume of hydrates over the pipeline's operational timeline is valuable for planning maintenance and intervention strategies. This helps maintain energy system reliability and sustainability by preventing unexpected disruptions.

Author Contributions: Conceptualization, O.M.U. and S.Z.I.; Methodology, O.M.U.; Software, O.M.U.; Validation, O.M.U.; Investigation, O.M.U.; Data curation, O.M.U.; Writing – original draft, O.M.U.; Writing – review & editing, S.Z.I., M.H. and A.K.; Visualization, O.M.U.; Supervision, S.Z.I., M.H. and A.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: The study did not require ethical approval.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Acknowledgments: The authors are grateful to the School of Engineering, Robert Gordon University, Aberdeen, United Kingdom, for supporting this research.

Conflicts of Interest: The authors declare no conflict of interest.

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