

Performance Comparison of Empirical and Semi-empirical Compressor Models with Uncertainty Analysis and Probabilistic Forecasting Techniques

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ABSTRACT

There are various empirical and semi-empirical models to estimate the performance of compressors. While some studies support the use of empirical methods for their high accuracy with the available experimental observations of compressor performance, others claim that semi-empirical methods can estimate the performance at extrapolation conditions more reliably. To understand if these claims are true, quantitative comparison of various types of compressor models was conducted based on uncertainty analysis. But these methods evaluate the accuracy and uncertainty of the models separately, and it is difficult for model users to comprehend their results. In this paper, the comparison of model accuracy and model uncertainty is combined together using a scoring method for probabilistic forecasting methods called interval score. The calculation of interval scores is widely used in the meteorological field to compare the accuracy of weather models with uncertainty outputs. This study uses interval scores of different compressor mass flow rate models to compare the performance five different empirical and semi-empirical compressor models with data from two compressors. The results of the comparison show that the most reliable model is a model that does not use redundant empirical coefficients nor physical principles, but even the most reliable model may fail to explain the compressor performance well under extrapolation.

1. INTRODUCTION

There are three main categories of compressor models to facilitate different applications: physical (white-box) models, empirical (black-box) models and semi-empirical (gray-box) models (Rasmussen, 2000). Physical models are developed based on basic physical principles such as mechanics, kinematics, thermodynamics and heat transfer to describe the compression of vapor inside a compressor. They are developed to improve compressor design processes by reducing time for unnecessary prototyping and testing of bad compressor designs. Empirical models are built based on empirical equations with few physical principles for fast computation of compressor performance. They contain empirical parameters that are estimated by regression based on observations of compressor performance (training data) under different operating conditions. One example is the commonly used 10-coefficient map of compressors which are cubic equations of evaporating temperature and condensing temperature in the ANSI/AHRI Standard 540-2004 (AHRI, 2004). Their simple structure and computation help engineers to design equipment using different compressors quickly. Semi-empirical models are modification of empirical models by adding mathematical expressions of some simple physical principles into empirical models. Although they contain fewer empirical parameters than empirical models and are often less accurate than empirical models at the training data points, their developers claim that semi-empirical models are less likely to overfit than empirical models and perform better at conditions outside the given experimental conditions (Jähnig et al., 2000).

Overfitting is an issue related to the use of a complex model that fit equally well as other simpler models (Hawkins, 2004). Overfit models may show higher accuracy at training data points, but their uses of more independent variables and empirical parameters than their counterparts may add random variation to their behavior and result in poor accuracy during extrapolation. Extrapolation is the use of a model to predict with data points that are not within the

range of data in the model's training data set. Hawkins (2004) demonstrated that the prediction error of a quintic polynomial during extrapolation can be much more severe than that of a linear equation despite the better prediction accuracy of the quintic polynomial at the training data points. Cawley and Talbot (2010) also described how overfitting of a machine learning algorithm would cause similar issues in a classification problem during extrapolation. These studies showed that overfitting weakened a model's ability to extrapolate appropriately.

Similar studies were also conducted for compressor models. Jähnig et al. (2000), Li (2012) and Aute et al. (2015) used extra testing data to investigate if accuracy of compressor models is worsened at extrapolation. While Jähnig et al. (2000) and Li (2012) found that the semi-empirical models perform better at extrapolation, Aute et al. (2015) showed otherwise with a much larger data set. To comprehensively describe the issue, uncertainty analyses were carried out in addition to these accuracy-based studies. Aute et al. (2016) and Cheung et al. (2017) studied the change of uncertainty of the AHRI 10-coefficient map as the compressor model extrapolates and found that the extrapolation issue can be mitigated by appropriate choices of training data. Cheung and Wang (2018) compared the uncertainty of empirical and semi-empirical models of compressor mass flow rates and found that both empirical and semi-empirical models can overfit when they become too complex and result in large uncertainty at their outputs.

While these studies provided separate views of the extrapolation issue of empirical and semi-empirical compressor models in terms of model accuracy and uncertainty, they failed to provide a more comprehensive picture as demonstrated in other areas that use probabilistic forecasting techniques. For example, probabilistic weather forecast models were evaluated based on performance metrics calculated from both accuracy and uncertainty (Gneiting and Raftery, 2007). Similar techniques were used to evaluate electricity pricing forecast models (Weron, 2014). To compare the overall performance of empirical and semi-empirical compressor models under extrapolation conditions, model evaluation techniques for probabilistic forecasting models should be used.

In this paper, interval scores that evaluate probabilistic forecasting models are calculated from various types of compressor models to compare the overall performance of empirical and semi-empirical models of compressors. The second section of the paper describes the evaluation method of the models using the interval scores, and the third section describes the five compressor mass flow rate models and two sets of compressor data being used in this study. The forth section evaluates the results of the evaluation, including the accuracy, uncertainty and interval scores of the compressor models, to examine if the use of physical principles can lessen the overfitting issue and improve the model's performance under extrapolation.

2. MODEL EVALUATION METHOD

To compare the accuracy and uncertainty of various compressor models, their empirical parameters should first be estimated by nonlinear regression. After that, the uncertainty calculation method developed in Cheung and Wang (2018) is used to estimate the uncertainty values under various compressor operating conditions. The interval scores of the models can be calculated based on the accuracy and uncertainty at these conditions to compare the performance of the models.

2.1 Nonlinear regression

Both empirical and semi-empirical models contain empirical parameters. Ideally, they can be described as Equation (1).

$$y_{true} = f(\vec{x}_{true}, \vec{\beta}_{true}) + \varepsilon \quad (1)$$

Equation (1) shows how a nonlinear regression equation based on vectors of true values of independent variables and empirical parameters can be used to give the true values of a dependent variable with an error term in an ideal situation. But true values of any variable cannot be obtained in reality, and the prediction of a dependent variable by nonlinear regression is conducted by Equations (2) and (3).

$$y_{pred} = f(\vec{x}_{mea}, \vec{\beta}_{pred}) \quad (2)$$

$$\vec{\beta}_{pred} = g(\mathbf{X}_{train}, \vec{y}_{train}) \quad (3)$$

Equation (2) shows how a non-linear regression uses measured values of independent variables and predicted values of empirical parameters to estimate a dependent variable. The predicted empirical parameters are estimated by Equation (3) using multiple measurement of independent variables and dependent variables in a set of training data. Nonlinear optimization methods are used to estimate the empirical parameters in Equation (3) so that the objective function in Equation (4), which is the sum of squares of deviations between the estimated and measured dependent variable at the training data points, is minimized (Nocedal and Wright, 2006).

$$J = \sum_i \left(y_{train,i} - f(\vec{x}_{train,i}, \vec{\beta}_{pred}) \right)^2 \quad (4)$$

2.2 Uncertainty calculation method of nonlinear regression models

The uncertainty of nonlinear regression model Equation (1) can be estimated by calculating the 95% confidence interval of the predicted dependent variable as shown in Equation (5) (Cheung and Wang, 2018).

$$\Delta y_{pred} = t_{n_{train}-q, 0.95} \sqrt{\Delta y_{input}^2 + \Delta y_{output}^2 + \Delta y_{train}^2 + \Delta y_{model}^2 + \Delta y_{num}^2} \quad (5)$$

There are 5 uncertainty components in Equation (5): uncertainty due to inputs, uncertainty due to outputs, uncertainty due to training data, uncertainty due to model random error and uncertainty due to numerical method. For simplicity, this paper only includes the definition of the components. The mathematical details to calculate them can be found in Cheung et al. (2017) and Cheung and Wang (2018).

2.2.1 Uncertainty due to inputs: Measured independent variables in Equation (1) carry measurement uncertainties such as sensor uncertainty and noise from the experimental environment. They propagate to form a part of the uncertainty of the estimated dependent variable in Equation (1) as demonstrated in Kline and McClintock (1953).

2.2.2 Uncertainty due to outputs: Equation (3) uses measured values of dependent variables to estimate the empirical parameters, and the uncertainty of the estimated dependent variable in Equation (1) calculated from other sources is its uncertainty to the measured value of the dependent variable. However, the uncertainty calculated from Equation (5) should be the uncertainty of the dependent variable to its true value. Hence an uncertainty component that describes the uncertainty between the measurement of the dependent variable and its true value should be introduced, and this is the uncertainty due to outputs.

2.2.3 Uncertainty due to training data: Training data in Equation (2) are collected by similar methods as the measured independent variables in Equation (1), and they carry similar type of uncertainties. Their uncertainties should therefore be propagated to the estimated dependent variable in Equation (1) through the estimation function of the empirical parameters in Equation (2) using the method in Kline and McClintock (1953) as well.

2.2.4 Uncertainty due to model random error: The training data set in Equation (2) is only a subset of all possible independent and dependent variables in the entire applicable range of Equation (1). It can never be certain if the selection of training data in Equation (2) can account for the relationship of all possible pairs of independent and dependent variables. Even if the whole population of independent and dependent variables in the applicable range of Equation (1) is used to estimate the empirical parameters in Equation (2) and the estimates of the empirical parameters equal to their true values, there is always an uncertainty in the estimate of the regression equation due to the error term in Equation (1). These two sources of uncertainties form uncertainty due to model random error.

2.2.5 Uncertainty due to numerical method: Since the estimation of empirical parameters in Equation (2) involves the use of numerical optimization methods, the effect of the uncertainty of numerical method to the estimated dependent variable should be calculated. Results of numerical optimization may change due to the uses of different threshold levels and different number of iterations, and this forms uncertainty in the empirical parameters. The uncertainty of the empirical parameters due to different threshold levels can be calculated by the Eigenvalue method (Oberkampf and Roy, 2010), and the uncertainty of the empirical parameters due to different number of iterations can be calculated by Richardson extrapolation (Oberkampf and Roy, 2010).

2.3 Calculation of interval scores

Interval score of a nonlinear regression model is a performance metric to rate the model's performance based on the model's accuracy and uncertainty. It can be calculated after the estimation of the empirical parameters. At a given data point, the accuracy of the model can be rated based on the deviation between the estimated and measured dependent variable, and its uncertainty can be calculated based on the confidence interval of the estimated dependent variable. The deviation and uncertainty can be used to calculate the interval score as shown in Equation (6) (Gneiting and Raftery, 2007).

$$S_{1-\alpha}(y) = \frac{2\Delta y_{pred}}{\alpha} + \frac{2}{\alpha} (y_{pred} - \Delta y_{pred} - y_{mea}) \cdot \mathbb{I}((y_{pred} - \Delta y_{pred}) - y_{mea}) + \frac{2}{\alpha} (y_{mea} - (y_{pred} + \Delta y_{pred})) \cdot \mathbb{I}(y_{mea} - (y_{pred} + \Delta y_{pred})) \quad (6)$$

where $\mathbb{I}(x)$ is a step function which equals to 1 if x is greater than 0 and equals to 0 for all other cases.

Equation (6) shows the mathematical function used to calculate an interval score. Its minimum value is the magnitude of the confidence interval which accounts for the effect of uncertainty on the performance of the model. It also depends on the difference between the measured value of the dependent variable and the lower and upper bounds of the confidence interval. If the measured dependent variable lies outside the confidence interval, the interval score will become larger than the confidence interval. This lowers the rating of a model for its failure to account for the behavior of the dependent variable within the model uncertainty and for potential significant systematic biases in the model. Hence a model performs better at a data point when its interval score is lower.

2.4 Evaluation using interval scores

Because a smaller interval score means a better model estimate, the model yields the smallest interval scores within the applicable range of a model should be the best model among all models being selected. The distribution of interval scores for each model at the available data points should also be evaluated to examine if a model is subjected to serious overfitting issues and extrapolation errors.

3. MODEL AND TEST DATA SELECTED FOR CASE STUDY

To examine if the number of empirical parameters and physical principles affect the model performance rated by interval scores, five compressor flow rate models with different number of physical principles are selected. They are applied to estimate the compressor mass flow rates of two compressors using the same set of training data. The interval scores of the compressor mass flow rate models at different operating conditions will be compared.

3.1 Compressor mass flow rate models

The five compressor mass flow rate models chosen for the study are the 10-coefficient compressor map with adjustment for compressor inlet superheat (Model I) (AHRI, 2004; Dabiri and Rice, 1981), a model with volumetric efficiency estimated by a quadratic polynomial (Model II) (Rasmussen, 2000), a model based on adiabatic compression (Model III) (Jähnig et al., 2000), a model based on adiabatic compression and back leakage loss (Model IV) (Arora, 2009) and a model based on isentropic compression (Model V) (Zakula et al., 2011). They are selected because they have the same dependent variable (compressor mass flow rate) and independent variables (compressor suction temperature, compressor suction pressure and compressor discharge pressure) but different number of empirical parameters and physical principles. Their differences of the number of empirical parameters and physical principles are tabulated in Table 1.

Table 1: Summary of the number of empirical parameters and physical principles in the models

Model	Number of empirical parameters	Physical principles involved
I	11	a. Tuning of mass flow rate by compressor suction density
II	6	a. Definition of compressor volumetric efficiency
III	3	a. Definition of compressor volumetric efficiency b. Adiabatic compression c. Compressor suction pressure loss
IV	4	a. Definition of compressor volumetric efficiency

		b. Adiabatic compression c. Compressor suction pressure loss d. Compressor back leakage loss
V	3	a. Definition of compressor volumetric efficiency b. Isentropic compression c. Compressor suction pressure loss

The equations of the compressor mass flow rate models are listed in the Appendix for reference. The uncertainty calculation method and the method to estimate the empirical parameters can be found in Cheung and Wang (2018).

3.2 Experimental data of compressors

To test the models in Table 1, some observations of compressor performance are needed. This study utilized laboratory testing data from two compressors as shown in Table 2 (Shrestha et al., 2013a and 2013b).

Table 2: Specification of compressors

	Compressor 1	Compressor 2
Type	Hermetic scroll	Hermetic scroll
Displacement volume	20.3 cm ³ rev ⁻¹	51.0 cm ³ rev ⁻¹
Rated power consumption	2.17 kW	3.32 kW
Rated mass flow rate	0.0396 kg/s	0.0624 kg/s
Refrigerant	R410A	R404A

The compressors were tested in Shrestha et al. (2013a, 2013b) following the ANSI/ASHRAE Standard 23.1-2010 (AHRI, 2010) in calorimeters. They were tested under different compressor suction and discharge dewpoint and compressor suction temperature as shown in Figure 1.

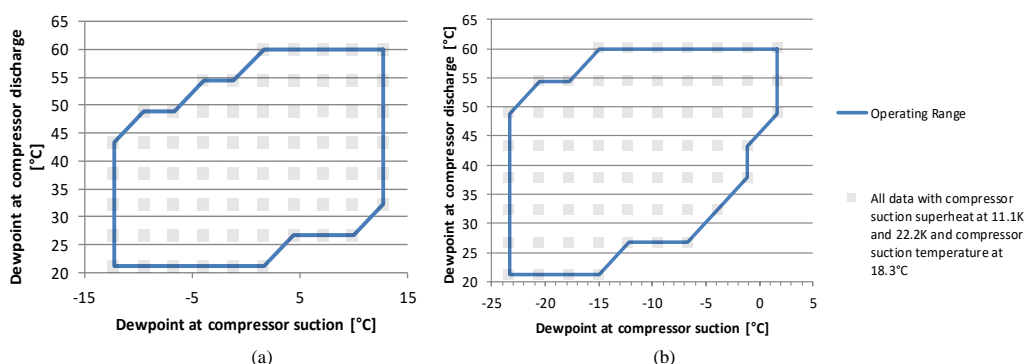


Figure 1: Operating conditions of (a) Compressor 1 and (b) Compressor 2 during laboratory tests

During each test, the temperature of compressor suction and discharge were measured by resistance temperature detectors with accuracy at $\pm 0.2\text{K}$. Coriolis mass flow meters were used to measure the compressor mass flow rate with accuracy at $\pm 0.1\%$, and refrigerant pressure at compressor suction and discharge were also measured with accuracy at $\pm 0.25\%$ of their full measurement scale. Other details of the measurement can be found in Shrestha et al. (2013a, 2013b).

To select the training data from the compressor testing data, the rule of thumbs to create model I in the compressor industry is used (Aute et al., 2015). The operating conditions of the training data set of each compressor are shown in Figure 2.

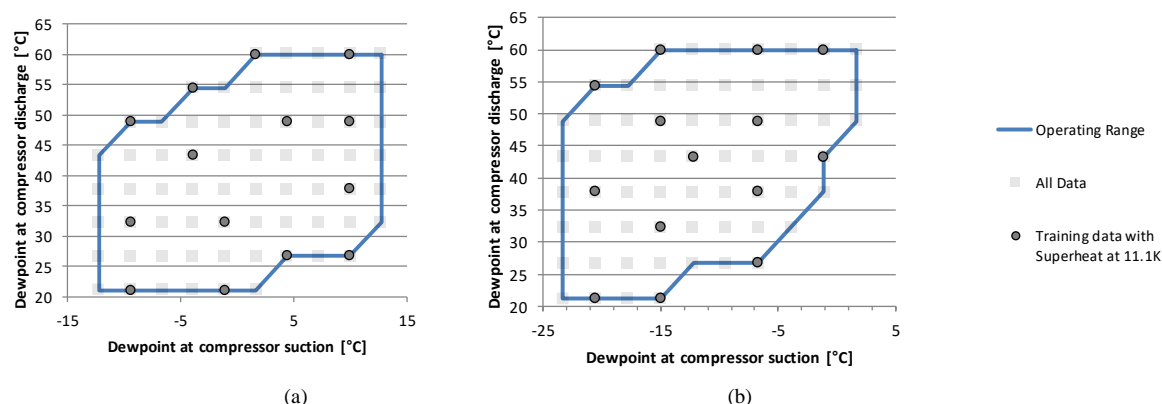


Figure 2: Training data of (a) Compressor 1 and (b) Compressor 2

Figure 2 shows that the training data are selected so that they cover the entire operating range of the compressors. There are also 14 data points in the training data only (Aute et al., 2015). The rule of thumb is to minimize the number of observations needed to quantify the compressor performance by Model I that has 11 empirical parameters, and the number of training data points must be greater than the number of empirical parameters in a model.

4. RESULTS AND DISCUSSION

4.1 Comparison of accuracy of the models

Accuracy of the models at all data points in Figure 1 are quantified by relative deviations. Relative deviations are calculated by dividing the difference between the measured and the estimated compressor mass flow rates by the measured mass flow rate. The smaller the magnitude of the relative deviations of a model, the higher its accuracy. Traditionally, the accuracy of models is only evaluated at training data points to minimize the number of measurement. The relative deviations of the models at the training data points are shown in Figure 3.

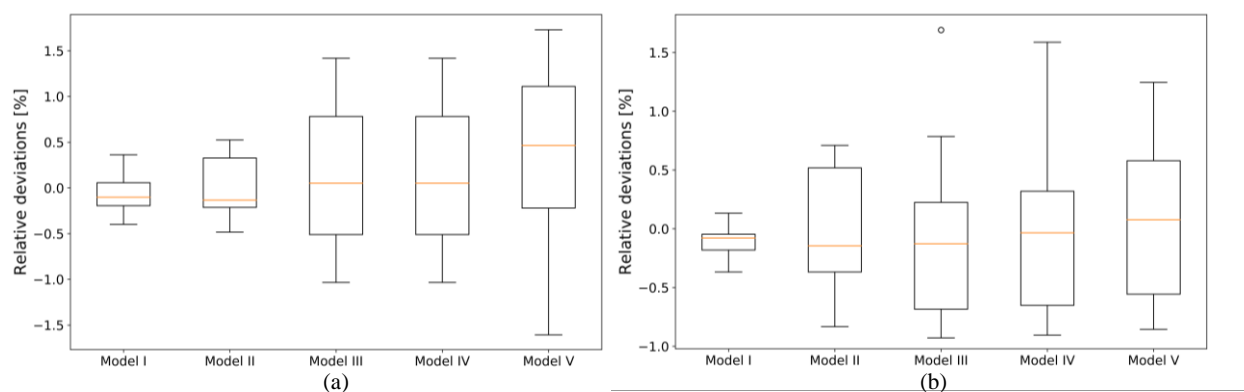


Figure 3: Box plots of models' relative deviations at training data points in Figure 1 for (a) Compressor 1 and (b) Compressor 2

Figure 3 shows that the Model I is the most accurate model, and model accuracy is lowered as the model contains fewer empirical parameters and more physical principles. However, this is actually caused by overfitting because the observation cannot be found in Figure 4 where the relative deviation at all data points in Figure 1 are visualized.

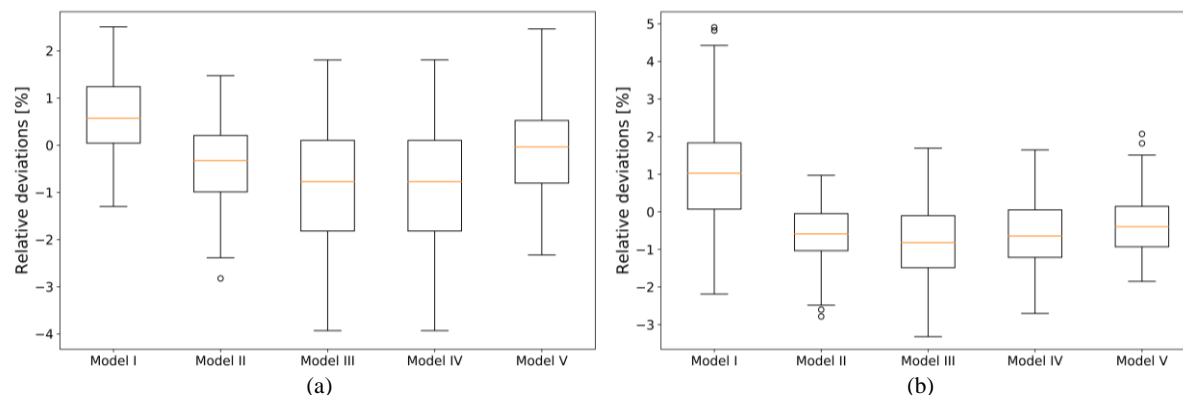


Figure 4: Box plots of models' relative deviations at all data points in Figure 1 for (a) Compressor 1 and (b) Compressor 2

Figure 4 evaluates the performance of the models by checking the accuracy of the model at all data points and finds that Models II and V are more accurate than other models for both Compressors 1 and 2.

4.2 Comparison of uncertainty of the models

Uncertainties of the models are compared to analyze the effect of measurement randomness and incomprehensiveness of training data to their performance. The evaluation is conducted using relative uncertainties calculated by dividing the uncertainty of predicted mass flow rate by the magnitude of the prediction. The larger the relative uncertainty, the more the model is subjected to the randomness and incomprehensiveness of measurement, and the worse its performance is. The relative uncertainties for each model are visualized in Figure 5.

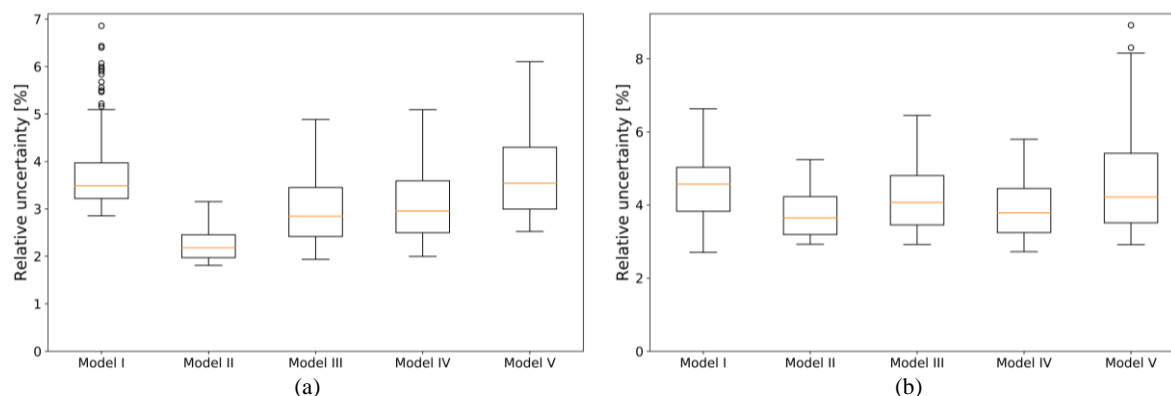


Figure 5: Box plots of models' relative uncertainties at all data points in Figure 1 using data from (a) Compressor 1 and (b) Compressor 2

Figure 5 shows that Model II is less subjected to randomness and incomprehensiveness of the training data than other models in the prediction of mass flow rates of Compressor 1. In the case of Compressor 2, Models II and IV predict mass flow rates more reliably than other models. This shows that more empirical parameters nor more physical principles can guarantee a better model performance. An accurate and reliable model should be built with appropriate number of physical principles and empirical parameters.

4.3 Comparison of the interval scores of the models

To evaluate the accuracy and uncertainty of a model with one performance metric, interval scores of the models are compared. Similar to the other metrics, interval scores calculated at each data point in Figure 1 can be normalized by the predicted mass flow rates. The distributions of the relative interval score for each model are plotted in Figure 6.

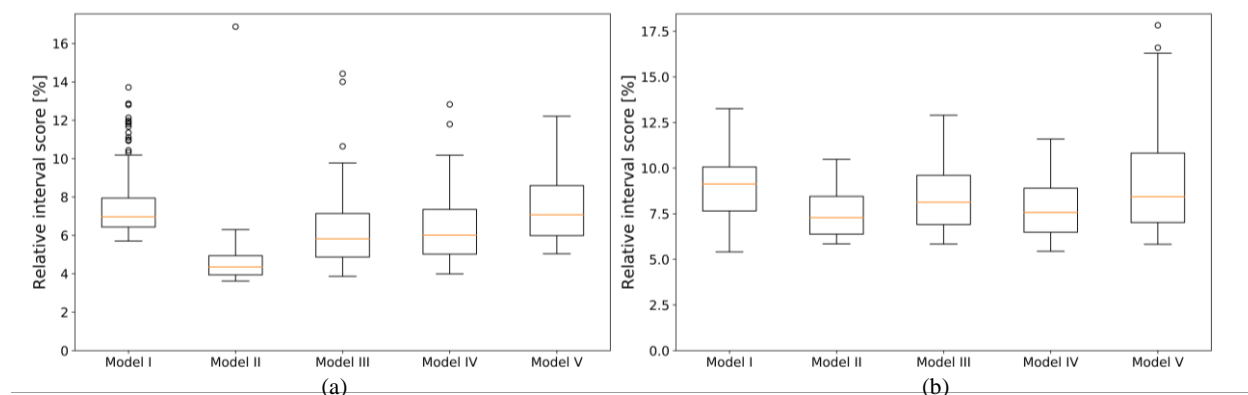


Figure 6: Box plots of models' relative interval scores at all data points in Figure 1 for (a) Compressor 1 and (b) Compressor 2

The results show a similar conclusion as other analyses that Model II is better than other models. However, it shows that the worst prediction comes from Model II too, in contrast to the conclusions of Figure 4 and Figure 5 which show that Model II estimate all mass flow rates with good accuracy and low uncertainty. Because the uncertainty of Model II is small, any inaccurate prediction is potentially a result of systematic error in the model. Hence interval score penalizes estimation deviation in Model II much more heavily than other models with larger uncertainties. Similarly, high interval scores are also found for Models III and IV in Compressor 1, showing that there are deficiencies in the models to explain the change of mass flow rate with its operating conditions. An in-depth analysis reveals that the large interval scores in these models all occur at data points with high superheat, showing that the use of compressor volumetric efficiency to account for mass flow rates in high superheat scenarios may not be as good as expected. Training data at high superheat situation may be necessary to account for the effect of high superheat effectively.

5. CONCLUSIONS

To conclude, this study shows how scoring rules for probabilistic approaches can be used to compare the empirical and semi-empirical compressor models. The accuracy and uncertainty of five empirical and semi-empirical models are evaluated using an accuracy metric, an uncertainty metric and a metric for probabilistic forecasting methods. Their evaluations show that higher number of empirical parameters nor number of principles can guarantee better extrapolation performance. The metric for probabilistic forecasting methods further shows that physical principles may not work to avoid model systematic bias at extreme operating conditions such as high superheat situation. Training data at high superheat situation may be needed even for semi-empirical models to model the effect of high superheat appropriately.

NOMENCLATURE

α	Type I Error	
β	Empirical parameter	
Δy	Uncertainty of variable y	(Follow variable y)
ε	Error in regression equation	
f	Function of model	
g	Function of model empirical parameter estimation	
J	Objective function	
\dot{m}	Mass flow rate	(kg/s)
n	Number of data points	
P	Pressure	(Pa)
ρ	Density	(kg/m ³)
s	Entropy	(kJ/kg-K)
S(y)	Interval score of variable y	(Follow variable y)
t	Student t-statistics	
T	Temperature	(°C)
x	Independent variable	(varies)

y	Dependent variable	(varies)	
Subscript			
dew	dewpoint	model	model random error
dis	compressor discharge	num	numerical method
input	input	output	output
I	Model I	pred	predicted
II	Model II	suc	compressor suction
III	Model III	true	true value
IV	Model IV	V	Model V
mea	measured		

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APPENDIX: MATHEMATICAL FORMS OF MASS FLOW RATE MODELS

A.1 Model I

Model I is the 10-coefficient compressor mass flow rate model from ANSI/AHRI Standard 540-2004 (AHRI, 2004) adjusted for the compressor inlet superheat (Dabiri and Rice, 1981) as shown in Equation (7).

$$\begin{aligned} \dot{m}_{comp,pred,I} = & \left(1 + \beta_{pred,I,10} \left(\frac{\rho_{suc}(T_{suc}, P_{suc})}{\rho_{suc, rat}(P_{suc})} - 1 \right) \right) (\beta_{pred,I,0} + \beta_{pred,I,1} T_{dew,suc} + \beta_{pred,I,2} T_{dew,dis} \\ & + \beta_{pred,I,3} T_{dew,suc}^2 + \beta_{pred,I,4} T_{dew,suc} T_{dew,dis} + \beta_{pred,I,5} T_{dew,dis}^2 + \beta_{pred,I,6} T_{dew,suc}^3 \\ & + \beta_{pred,I,7} T_{dew,suc}^2 T_{dew,dis} + \beta_{pred,I,8} T_{dew,suc} T_{dew,dis}^2 + \beta_{pred,I,9} T_{dew,dis}^3) \end{aligned} \quad (7)$$

where $\rho_{suc, rat}(P_{suc})$ is obtained with a rated compressor suction superheat at 11.1K and the dew point temperature values are estimated from the measured pressure at compressor suction and discharge.

A.2 Model II

Model II is a model which is built based on the definition of compressor volumetric efficiency which the volumetric efficiency is estimated by a quadratic equation of compressor suction and discharge temperature (Rasmussen, 2000). Its mathematical form is Equation (8).

$$\begin{aligned} \dot{m}_{comp,pred,II} = & \rho_{suc}(T_{suc}, P_{suc}) (\beta_{pred,II,0} + \beta_{pred,II,1} T_{dew,suc} + \beta_{pred,II,2} T_{dew,dis} + \beta_{pred,II,3} T_{dew,suc}^2 \\ & + \beta_{pred,II,4} T_{dew,suc} T_{dew,dis} + \beta_{pred,II,5} T_{dew,dis}^2) \end{aligned} \quad (8)$$

A.3 Model III

Model III is the model in Jähnig et al. (2000) as shown in Equation (9).

$$\begin{aligned} \dot{m}_{comp,pred,III} = & \beta_{pred,III,0} \rho_{suc}(T_{suc}, P_{suc}) \left(1 - \beta_{pred,III,1} \left[\left(\frac{P_{dis}}{P_{suc}(1 - \beta_{pred,III,2})} \right)^{(c_v(T_{suc}, P_{suc})/c_p(T_{suc}, P_{suc}))} - 1 \right] \right) \end{aligned} \quad (9)$$

A.4 Model IV

Model IV is modified from Equation (9) by adding a term explaining back leakage loss in a compressor to create Equation (10) (Arora, 2009).

$$\begin{aligned} \dot{m}_{comp,pred,IV} = & \beta_{pred,IV,0} \rho_{suc}(T_{suc}, P_{suc}) \left(1 - \beta_{pred,IV,1} \left[\left(\frac{P_{dis}}{P_{suc}(1 - \beta_{pred,IV,2})} \right)^{(c_v(T_{suc}, P_{suc})/c_p(T_{suc}, P_{suc}))} - 1 \right] \right. \\ & \left. - \beta_{pred,IV,3} \left(\frac{P_{dis}}{P_{suc}} \right) \right) \end{aligned} \quad (10)$$

A.5 Model V

Model V is modified from the model of compressor in Zakula et al. (2011) and describes the compression process as an isentropic compression. The equations in the model are listed from Equation (11) to Equation (13).

$$\dot{m}_{comp,pred,V} = \beta_{pred,V,0} \rho_{suc}(T_{suc}, P_{suc}) \left(1 - \beta_{pred,V,1} \left[\left(\frac{P_{dis}}{P_{suc}(1 - \beta_{pred,IV,2})} \right)^{(1/e_{is})} - 1 \right] \right) \quad (11)$$

$$e_{is} = \frac{\ln \left(\frac{P_{dis}}{P_{suc}} \right)}{\ln \left(\frac{\rho_{dis,s}}{\rho_{suc}} \right)} \quad (12)$$

$$\rho_{suc} = \rho(P_{dis}, s = s(T_{suc}, P_{suc})) \quad (13)$$