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Non-linear relationship between combustion kinetic parameters and coal quality

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Abstract: Combustion kinetic parameters (i.e., activation energy and frequency factor) of coal have been proven to relate closely to coal properties; however, the quantitative relationship between them still requires further study. This paper adopts a support vector regression machine (SVR) to generate the models of the non-linear relationship between combustion kinetic parameters and coal quality. Kinetic analyses on the thermo-gravimetry (TG) data of 80 coal samples were performed to prepare training data and testing data for the SVR. The models developed were used in the estimation of the combustion kinetic parameters of ten testing samples. The predicted results showed that the root mean square errors (RMSEs) were 2.571 for the activation energy and 0.565 for the frequency factor in logarithmic form, respectively. TG curves defined by predicted kinetic parameters were fitted to the experimental data with a high degree of precision.

Key words: Kinetic parameter, Coal property, Thermo-gravimetry (TG), Support vector regression machine (SVR), Differential evolution

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1 Introduction

Coal utilization requires a good understanding of the combustion characteristics of coal. The relationship between the combustion characteristics and the coal properties has been widely investigated. Firstly, the ignition behavior is affected by the coal properties. The ignition order generally follows the coal rank (Man and Gibbins, 2011), and the mechanism of ignition changes from heterogeneous to homogeneous for subbituminous coal and high volatile bituminous coal, respectively (Faúndez *et al.*, 2005). According to the experimental results of Kizgut and Yilmaz (2004), the ignition temperature shows an almost linear relationship with the mean maximum vitrinite reflectance (R_m), H/C ratio, and fuel ratio (the ratio of fixed carbon to volatile matter). The low volatility coal types require a slightly higher level of oxygen (35% O_2 (in volume) in CO_2) to give ignition patterns similar to those in air; whereas coal samples with high volatile matter require about 30% oxygen in general (Man and Gibbins, 2011). Ash content tends to increase the volumetric heat capacity, which slows the heating of coal particles, and thus delays ignition (Vleeskens and Nandi, 1986). Secondly, the maximum rate of mass loss in the thermo-gravimetry (TG) curve, which is an important indication of the reactivity of coal, is found to show a good linear relationship with R_m and H/C ratio (Kizgut and Yilmaz, 2004). Combustion experiments of 66 coal ranks, using derivative thermo-gravimetric analysis, showed that the temperature at which 50% of the samples achieve complete combustion has a linear relationship to the oxygen and carbon contents (Smith *et al.*, 1981). Finally, combustion efficiency is tied to coal properties. Experiments and theoretical research have been undertaken to investigate coal burnout. Results showed that the burnout increases with the decrease of fuel ratio (Du *et al.*, 2010) and that high volatile

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matter coal has a stronger devolatilization and therefore, a higher burnout (Shen *et al.*, 2009). Results also showed that high levels of ash, inertinite content, and oxidized vitrinite content can decrease burnout in a drop tube furnace (Vleeskens and Nandi, 1986).

The stages of the combustion process are characterized by different parameters. Ignition temperature represents the difficult degree of oxidation reaction at the early stage of burning. The maximum rate of weight loss reflects the intensity of the combustion reaction in the middle stage. Burnout temperature reflects the burnout performance of coal at the end of combustion. In fact, the combustion of coal can be considered as a first-order reaction (Cumming, 1984; Kök *et al.*, 1997; 2004; da Silva Filho and Miliol, 2008), and the reaction rate can be correlated with kinetic parameters by the Arrhenius equation. Therefore, the whole combustion process can be characterized by kinetic parameters. Some attempts have been made to explore the influence that coal properties exert on the combustion kinetics. Küçükbayrak *et al.* (2001) performed the non-isothermal TG experiments to investigate the combustion reactivities of 25 lignite samples. They related the combustion reactivity of the lignites to the proximate and ultimate analyses and the physical properties. The activation energy (E) tended to decrease as volatile matter content grew and increased as the content of total carbon or fixed carbon increased. Their further study of the combustion reactivity of different ranks of coal including peat, lignite, bituminous coal, and anthracite samples led to the same conclusion (Haykiri-Açma *et al.*, 2002). However, diametrically opposite results were manifested. Wang *et al.* (2010) conducted the experiments and showed that E decreased gently and frequency factor (A) decreased quickly with increasing carbon content in the coal.

The previous work on the burning characteristics of coal indicated that the combustion kinetics of coal is closely related to coal properties. However, the quantitative relationship between combustion kinetics and coal properties requires further study. In this paper, the combustion kinetic parameters (E and A) are correlated to coal quality such as proximate analysis and ultimate analysis. Thermo-gravimetric analyses of 80 coal samples were employed for the combustion kinetic study. A support vector regression machine (SVR) was used to build two non-linear models. Model-E is a model of the relationship between E and the coal quality; Model-A is a model of the relationship between $\ln A$ and the coal quality. Both models were validated using 70 training samples to evaluate empirical error and were tested on 10 holdout samples to mitigate model over-fitting. For assessing the generalization performance of the two models, kinetic parameters of the test samples were predicted using the two models together. TG curves of the test samples were calculated to manifest the prediction accuracy of the kinetic parameters.

2 Theoretical bases

SVR was developed on the statistical learning theory and has become a popular machine learning algorithm in many fields over the past decade years. With limited information from some training samples, SVR builds the model of the relationship between the output target and the input variables. SVR adopts a risk minimization principle in the modeling process; therefore, it has good inherent regularization properties to improve the generalization performance in the case of sparse data and large noise level (Müller *et al.*, 1997; Cherkassky and Ma, 2004). Besides, SVR has advantages in the assurance of global optimal solution (Iplikci, 2010) and the immunization against the problem of "dimension disaster" (Nizam *et al.*, 2010) over the conventional machine learning algorithms. The success of SVR is also due to the remarkable ability of handling non-linear high-dimensional problems (Cherkassky and Ma, 2004). The input data of non-linear systems are mapped into a high-dimensional feature space, and then a linear model can be constructed in this feature space (Balasundaram and Kapil, 2010). At the same time, the computation efficiency is enhanced by a kernel function that can replace the dot product in the feature space.

In this present analysis, the ε-insensitive loss function and radial basis function are used for the architecture of the SVR. Three tunable parameters exist: the insensitivity parameter ε, the regularization parameter C, and the kernel parameter γ. Because the SVR is very sensitive to the setting of the tunable parameters, the issue of assigning values to these parameters should be considered carefully. However,

no general technique of parameter selection is universally effective. The differential evolution (DE) algorithm is a heuristic method that addresses the purpose of minimizing possibly non-linear and non-differentiable functions (Storn and Price, 1995). It has advantages in suitability for parallelization, conceptual simplicity (Storn, 1996) and good convergence properties (Storn and Price, 1997). In this study, the DE algorithm is applied to the simultaneous search for the optimum values of the SVR parameters. The combination of SVR and DE is termed DE-SVR.

3 Experiments

3.1 Proximate and ultimate analyses

Eighty different coal samples were selected for investigation. Proximate and ultimate analyses were performed following China's National Standards GB/T 212-2008, GB/T 476-2008, GB/T 214-2007 and GB/T 19227-2008. The distribution characteristics with respect to volatile matter of the coal samples are described by a histogram as shown in Fig. 1. Extensive distribution of volatile matter (dry ash-free (daf) basis) from 7.61% to 56.19% (in mass) indicated that a large range of coal types was considered, from lignite to anthracite coal. The coal quality of the 80 coal samples can be found in Table A1 in Appendix.

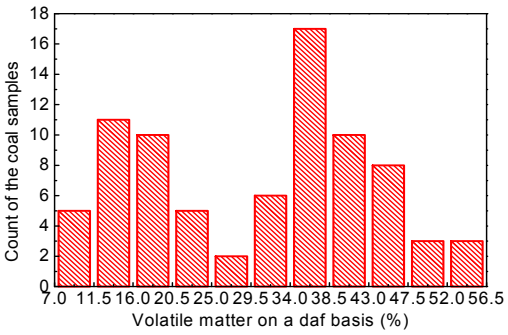

Fig. 1 Volatile matter distribution characteristics

3.2 TG experiments

Thermo-gravimetric analyses of the 80 coal samples were employed for the combustion kinetic study. A NETZSCH thermo-gravimetric analyzer TG 409 C was used. Each sample of 10 mg, ground to <90 μm in diameter, was placed in a thin layer in a porcelain crucible and heated from 50 to 1000 °C. The heating rate was 15 °C/min, and the air flow rate was 95 ml/min.

3.3 Calculation of the kinetic parameters

The parameters E and A of the coal samples were obtained from the kinetic analysis of TG data. The Coats-Redfern method has a great advantage of simplicity among the kinetic approaches and is extensively acknowledged (Jiang *et al.*, 2007; Avsar *et al.*, 2010; Janković, 2011; Kök, 2011a; 2011b; Liu *et al.*, 2011; Syed *et al.*, 2011; Wang *et al.*, 2011). When the sample size is small and the air supply is excessive, the progress of the reaction is independent of the oxygen concentration. It is therefore reasonable to assume that the oxidation can be described by first-order kinetics (Cumming, 1984; Kök *et al.*, 2004) and the Coats-Redfern equation (Coats and Redfern, 1965; Ebrahimi-Kahrizsangi and Abbasi, 2008), and therefore

$$\ln\left[-\frac{\ln(1-\alpha)}{T^2}\right]=\ln\frac{AR}{\beta E}\left(1-\frac{2RT_{\mathrm{m}}}{E}\right)-\frac{E}{RT}, \quad (1)$$

where α is the fractional conversion, T is the absolute temperature, β is the constant heating rate (15 °C/min), and T_{m} is the average of the absolute temperature of the fitting interval. For Eq. (1), the Arrhenius plot of the left side of the equation against $1/T$ results in a straight line. As a result, E can be calculated from the slope, and A can be calculated from the intercept. The kinetic parameters of all the 80 coal samples are listed in Table A1 in Appendix. The ranges were as follows: E=78.8 to 162.9 kJ/mol, and ln$A$=11.13 to 21.70 min^{-1}.

4 Training data and holdout data

Because the SVR may exhibit unsatisfactory performance on some tasks with a large range of values (Meyer *et al.*, 2003), each variable in the empirical data is scaled using Eq. (2) to unify the statistic distribution as follows:

$$X'=(X-X_{\min})/(X_{\max}-X_{\min}), \quad (2)$$

where X represents the variable to be scaled, and $X_{\max}$ and $X_{\min}$ are the maximum and minimum values of X, respectively.

Training data is used to guide the modeling process, while holdout data, which is absent in the

training process, carries novel information. The SVR models were built based on training data and were tested on holdout data. To this end, 70 coal samples were chosen uniformly from the 80 coal samples as training data, and the remaining coal samples were used as holdout data.

5 Application of DE-SVR

5.1 Key features affecting kinetic parameters

The coal quality parameters generally have unequal effect on the combustion kinetic parameters. Feature selection is intended to produce a low dimensionality of the input space and provide high prediction capability for the DE-SVR model. Different combinations of coal quality were studied to determine the key features. The following input features were manually determined: moisture on an air-dried basis (M_{ad}), fixed carbon on a dried basis (FC_d), volatile matter on a daf basis (V_{daf}), and hydrogen and sulfur contents on a dried basis (H_d and $S_{t,d}$). Therefore, the prediction of combustion kinetic parameters from coal quality can be represented by

$$E = f(M_{ad}, FC_d, V_{daf}, H_d, S_{t,d}), \quad (3)$$

$$\ln A = f(M_{ad}, FC_d, V_{daf}, H_d, S_{t,d}, E). \quad (4)$$

Considering the existence of the kinetic compensation effect (Koga and Tanaka, 1988; Koga and Sesták, 1991; MacCallum and Munro, 1992; Yip *et al.*, 2011) between E and $\ln A$, the calculated E is chosen as a sixth input feature, while the prediction model of $\ln A$ is trained using SVR.

5.2 Optimal models correlating kinetic parameters to coal quality

According to Eqs. (3) and (4), DE-SVR was applied to correlating the kinetic parameters and coal quality. The SVR parameters were optimized using the DE algorithm. It is necessary for the users to set the following three controlling variables of DE at the beginning: the size of the population NP, the scale factor F and the crossover probability CR. Some helpful rules (Storn, 1996; Storn and Price, 1997; Gämperle *et al.*, 2002; Ronkkonen *et al.*, 2005) have been summarized to instruct the users in setting the controlling variables correctly. The strategy DE/rand/1/bin (Storn, 1996; Storn and Price, 1997) with NP=100, F=0.7, and CR=0.85 was used in this study.

Optimum design of the SVR parameters corresponded to the minimization of the score function in the DE algorithm. In this study, the score of a candidate solution (i.e., the SVR parameters) was evaluated by using ten-fold cross validation (Kohavi, 1995; Salzberg, 1997) within the training data. The training data were further portioned into ten symmetrical subsets. Each of the ten subsets was used to test the model which was built by training on the remaining subsets. The test error was represented by the root mean squared error (RMSE) between the predicted and true kinetic parameters. The score was defined as the average value of the ten test errors. In this sense, the solution with the minimum score gave the optimal SVR parameters.

The established models will be appropriate for use as long as the optimal SVR parameters are used in the training progress. In this way, we built two optimal DE-SVR models named Model-E and Model-A. These models depicted the non-linear relationship between the combustion kinetic parameters and coal quality. Model-E and Model-A can be used as the prediction models for E and $\ln A$, respectively.

5.3 Validation of the optimal models

The accuracy of the DE-SVR models was validated with training data and holdout data. Predicted results are shown in Fig. 2. The predicted points of both the training data and the holdout data were approximately linear. In the case of validation using training data, the RMSEs for E and $\ln A$ were 2.707 and 0.143, respectively. The satisfactory model performance indicated that both of the DE-SVR models had low empirical errors and that the relationship between the combustion kinetic parameters and coal quality can be established using the DE-SVR models. In the case of validation using holdout data, the accurate prediction (RMSEs for E and $\ln A$ were 2.571 and 0.245, respectively) of the holdout data, with which the models had not been trained, implied the absence of over-fitting in the training process.

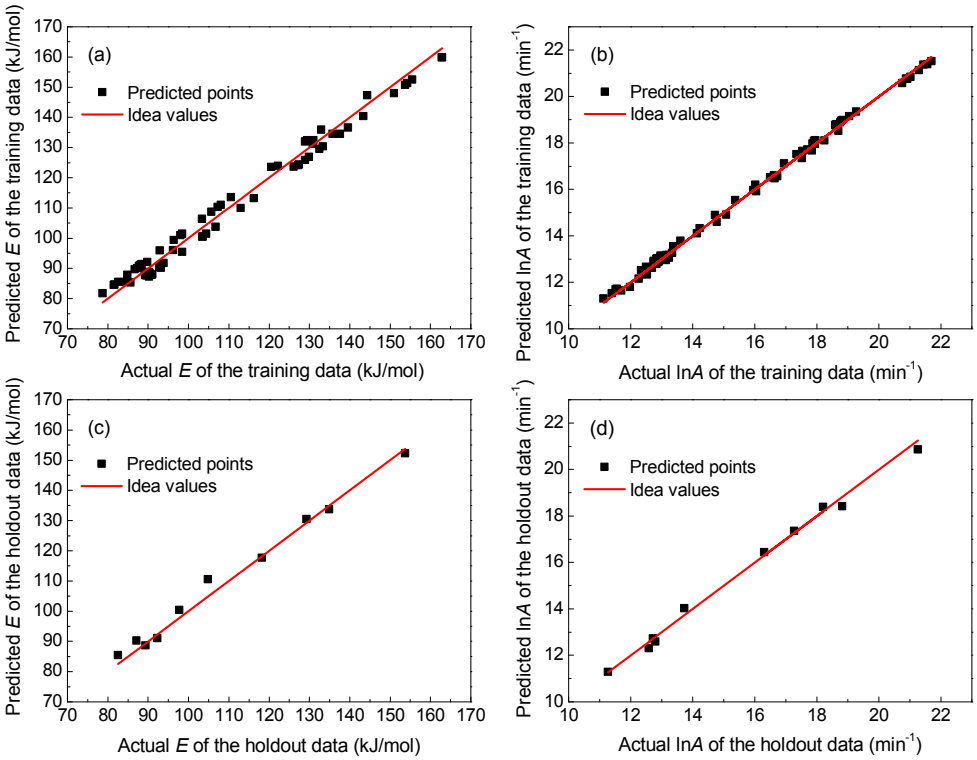

Fig. 2 Precision of the predicted kinetic parameters in the validation of Model-E and Model-A
(a) RMSE=2.707; (b) RMSE=0.143; (c) RMSE=2.571; (d) RMSE=0.245

6 Results

6.1 Prediction of the kinetic parameters

The ten coal samples in the holdout data were used as test samples for the two models. Considering that the kinetic parameters were unknown to the user in practice, the prediction was performed with the test samples using the models together, according to the manner in which the models will be applied in practice. Firstly, the value of E was predicted from Model-E, which reproduced identical results to those as shown in Fig. 2c. Additionally, the value of ln$A$ can be predicted from Model-A using the predicted value of E. The predicted results of ln$A$ are shown in Fig. 3. The difference between the RMSEs of Fig. 3 (0.565) and Fig. 2d (0.245) was small, which revealed that the predicted value of E could be used for the prediction of ln$A$. The predicted results of ln$A$ of the test samples indicated that the DE-SVR models had good generalization performance. Combustion kinetic parameters of novel coals can be accurately predicted from coal quality using the two models together.

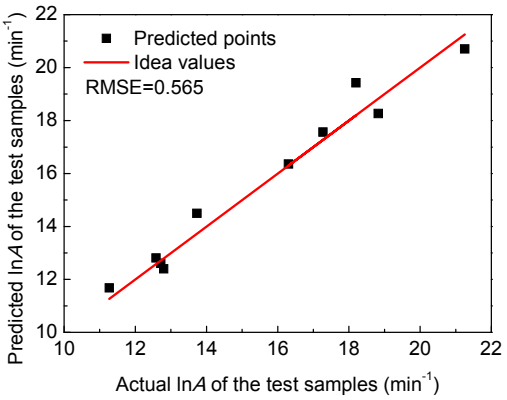

Fig. 3 Predicted ln$A$ of 10 test samples

6.2 Prediction of the TG curves

TG curves will allow us to measure the accuracy of the predicted kinetic parameters distinctly. According to Eq. (1), TG curves (300–700 °C, 5 °C step) could be determined by the predicted combustion kinetic parameters. The predicted TG curves of ten test samples deviated from the experimental data to different degrees. By using the experimental data as a

benchmark, the RMSE based on this deviation was calculated. The average and maximum RMSEs were 0.029 and 0.052, respectively. The overall fit between the predicted TG curves and the experimental TG data is shown in Fig. 4. The best results were obtained for sample 3, where the predicted TG curves fit the experimental data exactly. In sample 7, with moderate RMSE, the predicted TG curve deviated slightly from the experimental data. The maximum RMSE was observed for sample 9, where the accuracy of the fit of the predicted TG curve was acceptable. The overall fit between the predicted differential thermo-gravimetry (DTG) curves and the experimental DTG data of samples 3, 7, and 9 is shown in Fig. 5. These three different samples demonstrated that the predicted kinetic parameters were successful in determining the TG curves accurately. In other words, the combustion kinetic parameters based on the TG curves have been accurately predicted from the coal quality.

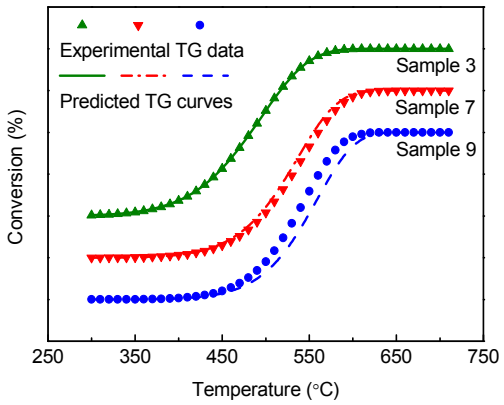

Fig. 4 Overall fit between the predicted TG curves and the experimental TG data of three typical samples

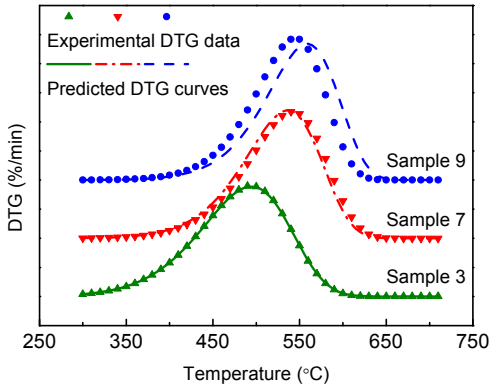

Fig. 5 Overall fit between the predicted DTG curves and the experimental DTG data of three typical samples

7 Conclusions

Kinetic analyses on TG data of 80 coal samples were performed to prepare sample data for the modeling of an SVR. The combustion kinetic parameters were correlated to the coal quality by the established DE-SVR models. The following conclusions can be drawn:

1. Validation results showed that both DE-SVR models had small empirical errors and were free of over-fitting.

2. Predicted results (RMSEs for E and $\ln A$ were 2.571 and 0.565, respectively) of the test samples showed that the DE-SVR models had good generalization performance.

3. The combustion kinetic parameters can be accurately predicted from the coal quality using the two DE-SVR models together.

4. Predicted TG curves, which were defined by the predicted kinetic parameters, fit the experimental TG data well.

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Appendix

The coal quality and kinetic parameters of all the 80 coal samples are listed in Table A1.

Table A1 Coal quality and kinetic parameters of the 80 coal samples

Sample	Coal quality (%)					Kinetic parameter	
	M_{ad}	FC_d	V_{daf}	H_d	$S_{t,d}$	E (kJ/mol)	ln$A$ (min^{-1})
Training data							
No. 1	5.4	46.51	49.99	3.06	1.60	78.8	12.52
No. 2	2.3	45.65	39.17	4.18	0.33	81.5	11.39
No. 3	2.7	51.87	33.35	3.16	0.65	81.7	11.13
No. 4	2.3	48.84	38.50	4.21	1.68	82.6	11.55
No. 5	2.4	51.05	33.19	2.91	0.68	84.1	11.51
No. 6	4.3	51.02	37.87	2.62	0.40	84.6	12.51
No. 7	3.0	53.03	34.73	4.08	0.51	84.9	11.98
No. 8	1.7	53.88	32.07	3.78	0.45	85.7	11.70
No. 9	3.9	44.70	43.83	4.46	1.14	86.7	13.13
No. 10	2.6	48.03	37.48	3.96	1.10	86.7	12.26
No. 11	3.2	45.61	39.63	4.10	0.73	87.3	12.33
No. 12	9.6	41.88	52.15	4.07	2.41	87.7	12.97
No. 13	6.0	36.00	54.08	3.26	0.60	87.9	13.61
No. 14	1.6	47.43	38.90	2.16	0.28	88.2	12.74
No. 15	2.7	54.95	36.24	4.83	0.88	88.5	12.49
No. 16	2.9	48.97	38.80	2.95	1.70	89.2	12.74
No. 17	2.4	39.68	43.04	2.96	0.24	89.3	12.84
No. 18	1.8	47.43	38.19	2.35	0.36	89.6	12.89
No. 19	4.4	50.05	37.40	3.73	1.27	89.8	12.83
No. 20	2.2	45.00	39.43	3.88	1.52	90.2	12.91
No. 21	1.9	41.48	42.91	3.80	0.39	90.2	12.96
No. 22	0.6	47.39	36.22	4.29	0.82	90.4	12.69
No. 23	2.4	50.32	37.03	4.21	0.73	90.9	12.87
No. 24	2.7	47.41	39.12	4.00	0.64	91.1	13.23
No. 25	3.3	51.74	35.90	3.80	0.97	92.8	13.18
No. 26	5.5	33.89	45.06	2.34	0.59	92.9	14.22
No. 27	3.6	51.60	36.18	3.79	1.25	93.1	13.14
No. 28	3.6	55.80	35.04	3.28	1.01	93.1	13.24
No. 29	3.3	54.99	35.18	3.82	1.00	93.8	13.33
No. 30	5.4	41.42	50.75	4.63	0.69	96.2	15.37

(To be continued)

(Table A1)

Sample	Coal quality (%)					Kinetic parameter	
	M_{ad}	FC_d	V_{daf}	H_d	$S_{t,d}$	E (kJ/mol)	ln$A$ (min^{-1})
Training data							
No. 31	3.9	29.33	40.64	2.81	0.36	96.4	14.77
No. 32	2.4	72.55	18.54	3.79	2.10	98.0	12.86
No. 33	3.3	48.85	28.40	3.24	2.53	98.5	13.38
No. 34	1.4	44.93	37.22	2.05	0.35	98.5	14.13
No. 35	17.2	45.28	46.98	5.91	0.33	103.4	18.60
No. 36	7.3	38.76	43.19	3.83	1.09	103.5	16.64
No. 37	6.3	33.43	40.80	3.04	0.32	103.5	15.96
No. 38	3.8	61.36	31.15	4.45	1.03	104.4	14.72
No. 39	9.4	53.21	35.70	3.19	0.34	105.7	16.02
No. 40	6.0	50.04	34.02	4.48	0.27	106.8	16.62
No. 41	11.4	46.43	44.68	4.58	0.25	107.3	18.79
No. 42	9.1	47.02	47.55	5.57	0.31	108.1	19.28
No. 43	2.2	58.37	20.73	3.13	2.15	110.6	15.08
No. 44	12.2	43.89	47.42	5.33	0.33	113.0	20.75
No. 45	1.8	58.19	21.81	3.01	1.84	116.3	16.04
No. 46	1.7	56.92	20.22	2.93	2.78	120.6	16.50
No. 47	1.3	45.16	17.91	1.92	0.85	122.2	16.73
No. 48	0.7	57.33	19.31	2.56	1.29	126.1	17.51
No. 49	2.3	57.12	19.52	2.89	2.59	127.2	17.35
No. 50	0.8	48.16	22.93	3.22	2.75	127.4	17.69
No. 51	2.2	61.32	17.36	3.08	2.39	128.9	17.53
No. 52	1.7	64.95	13.60	2.91	0.31	129.0	16.95
No. 53	1.3	47.08	21.34	2.75	2.97	129.5	17.87
No. 54	0.6	54.24	19.13	3.14	2.35	129.9	17.91
No. 55	1.6	67.04	14.65	3.07	0.72	130.8	17.84
No. 56	1.2	58.10	17.38	2.87	2.37	131.0	18.24
No. 57	12.1	58.65	56.19	4.55	0.42	132.5	21.70
No. 58	2.3	63.97	14.18	2.77	1.07	132.9	17.94
No. 59	2.1	61.24	15.21	2.90	0.53	133.4	17.95
No. 60	1.3	50.03	17.95	2.65	2.33	135.8	18.75
No. 61	1.7	68.64	13.54	3.17	0.29	137.6	18.70
No. 62	1.7	64.11	14.31	2.83	1.27	139.6	19.04
No. 63	2.1	69.73	11.41	2.67	3.18	143.4	18.82
No. 64	2.2	73.50	10.21	2.58	1.10	144.3	18.63
No. 65	1.2	67.36	11.78	3.66	0.51	151.0	20.88
No. 66	3.4	58.89	13.02	2.94	4.73	153.7	20.92
No. 67	3.2	51.67	15.15	2.49	3.77	154.3	21.02
No. 68	1.9	68.03	10.65	3.01	1.32	155.5	21.30
No. 69	3.3	66.28	9.50	2.55	0.75	162.8	21.44
No. 70	1.4	68.11	7.61	2.69	0.32	162.9	21.56
Holdout data (test samples)							
No. 71	1.9	53.98	32.77	3.88	0.46	82.5	11.27
No. 72	2.7	53.56	37.47	3.72	0.96	87.1	12.58
No. 73	2.5	49.14	38.16	4.31	0.88	89.4	12.72
No. 74	2.5	57.86	29.35	3.86	0.32	92.3	12.80
No. 75	3.9	60.08	33.31	4.59	0.88	97.7	13.73
No. 76	11.6	47.01	46.85	4.48	0.45	104.8	18.20
No. 77	1.0	47.13	21.19	3.26	0.79	118.2	16.31
No. 78	2.0	65.43	14.75	3.02	0.55	129.3	17.27
No. 79	0.6	61.45	18.39	3.18	4.27	134.9	18.82
No. 80	3.4	57.52	13.86	2.68	3.62	153.8	21.25