Simulation of Winter Durum Wheat Flour Yield Based on Structural Equation Modeling

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Abstract

Flour yield determined the profitability of flour mill, but the intrinsic variability of the grain makes it very complex to analysis and estimate wheat grain flour yield. Simulation for flour yield attributes offer considerable advantages in flour mill, if reliable predictions of flour yield can be provided, because the wheat grain characteristics can be tested before milling. If this is possible, the characteristics thus observed could be quantified more reliably and objectively by Structural Equation Modelling (SEM). SEM was used to look for the most important wheat grain characteristics on flour yield, and then these wheat grain characteristics were used to simulate flour yield. Furthermore, the regressive equation was verified by the field experiment. The coefficient of variation of grain characteristics was low and distributed rather closely. The results of SEM showed that test weight had the most significantly effects on flour yield, followed by the hardness index. Test weight and hardness index could excellently estimate flour yield by multiplicative effect of test weight and hardness index, and which could determine 68% of the variation in flour yield. The simulation result can not only predict flour yield, but also look for the important grain characteristics for the flour yield.

Key words: Flour yield; Winter durum wheat; Grain characteristics; Structural equation model; Simulation;

1. Introduction

Wheat is the largest cost for a flour mill, and profitability is determined mostly by flour yield(Doblado Maldonado et al., 2012). About 82-86% starchy endosperm was in the wheat grain, but only 76-78% could be separated(Edwards, 2010). The endosperm to bran ratio and ease of separation were the determinant of flour yield(Y and Z, 2001). The former was more affected by the grain shape, the thickness of the testa, depth and width of crease, and the size of the embryo; and the latter is related to the grain moisture content, hardness and density. But all of above had an inevitable relationship with flour yield.

Test weight was used as a quality parameter which may predict potential flour yield(Finney and Andrews, 1986), but most reaches think it was unreliable predictor(Ghaderi and Everson, 1971). It is generally acknowledged that there was a positive correlation between test weight and flour yield, but the significantly positive correlation only existed when the cultivar, site, and planting season were all the same. Hardness is also considered to be an essential factor for wheat flour yield(Haddad et al., 2001). Pomeranz(Pomeranz and Williams, 1990) even presented that hardness was the most important factor affecting flour yield. Comparing to test weight, hardness showed heredity stability(Lehmensiek et al., 2006). Moisture content, falling number, crude protein, test weight and hardness were all had affected on flour yield. Because of the contradictions of a large number of studies, the large samples data would be more credible and persuasive.

Despite the best efforts of breeders and farmers, wheat flour yield was variable, and little quantitative information was available(Dobraszczyk et al., 2002). But the flour yield is the comprehensive expression of grain characteristics, a single characteristic was difficult to reflect change of flour yield. The most research methods were multiple linear regression to reflect the law of flour yield which affected by grain characteristics(Mog, 2011) and puroindoline(Edwards, 2010), a nonlinear regression(Flores et al., 1991), or computer

simulation(Loza-Garay and Flores, 2003). But all of these simulated results were not very precise.

Generally, it is believed that genotype is the most important factor for wheat quality(Li et al., 2013); while Blumenthal et al(Blumenthal et al., 1993) propose that environment and management also play an important role in wheat milling quality. Wheat exhibits over 25,000 cultivars in a wide range of temperate environments(Jenkins, 2011). Although there are many studies on wheat milling quality, the research conclusions are limited by their specificity of time and space and cannot be applied generally in other regions.

The objectives of this paper were to: (a) analysis the winter durum wheat grain morphological; (b) identify the most important wheat grain characteristics for flour yield; (c) simulate flour yield by the identified grain characteristics.

2. Materials and Methods

2.1 Samples

The potential of this approach was investigated by examining 617 winter durum grain samples of about 69 cultivars from 2008 to 2016, which were collected from the Cereal Quality Supervision and Testing Center, Ministry of Agriculture, China(Cereal Quality Supervision Testing Center, 2016). The cultivars were medium gluten wheat and strong gluten wheat, which were from southern Hebei, northern Henan, central and northern Shandong, southern Shaanxi, northern Shaanxi and eastern Gansu (Fig. 1). And this area belongs to Northern part of Huang-huai Region, which is one of the ten wheat-quality regions of China. Annual precipitation in these areas is 400-800mm.

2.2 Experimental design

Field experiment was from 2014 to 2016 in Yangling, Shaanxi (34°14' N, 108°3' E, 506 m a.s.l.). Wheat cultivar was “*Xiaoyan 22*” (*Triticum aestivum* L.), which was winter durum wheat. Experimental design was a randomized complete block with a split-plot arrangement

and three replications. The whole plot factor was irrigation (4 levels) and the subplot was nitrogen fertilization (4 levels). The data of field experiment was used to verify the regression curve.

2.3 Grain analysis

The hardness index, test weight, moisture content, falling number, grain protein content (GPC), and flour yield were determined according to the GB/T 21304-2007 (Near infrared reflectance spectroscopy Instalab610, new port scientific sales and services pty Ltd, Australia), GB/T 5498-1985, GB/T 5497-1985, GB/T 10361-2008, GB/T 10361-2008 (Kjeldahl apparatus, JELTEC 2300, Sweden FOSS), and NY/T1094.2-2006 (Bühler MLU-202, Switzerland), respectively.

2.4 Data analyses

The samples data collected from Northern part of Huang-huai Region were used to find out the most important grain characteristics which affected flour yield, and quantify the relationship between most important grain characteristics and flour yield. The data based on the nitrogen fertilization and irrigation treatments was used to analysis effects of nitrogen fertilization and irrigation on milling quality, and validate the correctness of the formulas.

Data analyses were performed with SPSS v20. Analysis of variance (ANOVA) was performed using a general linear model. Duncan's multiple-range test was used to determine the significant difference between treatments ($p < 0.05$). Regression analysis was conducted to quantify the relationships of grain character with flour yield. Structural Equation Modeling (SEM) was used to further explore the causality by SPSS AMOS v20. It is a modern statistical method of path analysis, which allows for both the direct and indirect effects between networks of intercorrelated variables (Anderson, Gerbing, 1988). The comparative fit index (CFI) was used to assess the model fit. Non-significant paths from the model were removed gradually to

fit the samples. The effect of hardness index, test weight, moisture content, falling number, and crude protein on flour yield was analysed by SEM.

2.5 Validation of regressive equation

Model validation was through comparing to measured and simulated flour yield. The RMSD represents the sample standard deviation of the differences between predicted values and observed values. The result of validation was evaluated by the root-mean-square error (RMSE) and relative-root-mean-square-error (RRMSE). The data of 16 different irrigation and fertilization treatments from 2014- 2016 was used to validate parameters.

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (s_i - o_i)^2}{n}} \quad (1)$$

$$RRMSE = \frac{\sqrt{\frac{\sum_{i=1}^n (s_i - o_i)^2}{n}}}{\frac{\sum_{i=1}^n o_i}{n}} \times 100\% \quad (2)$$

In Eq. (1) and (2), s_i , is simulated value; o_i , is observed value; n , is the sample size. The smaller RRMSE, the smaller difference of measured and simulated values (0-10%, excellent; 10%-20%, good; 20%-30%, fair and >30%, poor).

3. RESULTS

3.1 Summery of the collected samples from the Northern part of Huang-huai Region

The data included hardness, test weight, moisture content, falling number, crude protein, and flour yield. The coefficient of variation (CV) was all less than 10%, except the CV of falling number which reached to 16.68% (Table 1). The CV of test weight, hardness index, moisture content, and crude protein were relatively small. Classification on regions based on wheat quality in China cannot reflect the change of falling number very well. Test weight, hardness index, moisture content, and crude protein were affected by environment. The minimum hardness index was only 37, which was up to the standard of soft wheat. And the

minimum crude protein was only 9.54 g/100g, also almost belonged to weak wheat. The mean values essentially belonged to white-hard-strong wheat (Peterson et al., 1997).

The hardness index and test weight mainly distributed 60-70 and 780-825 g/L, respectively (Fig. 2a, b). The hardness index and test weight were large and did not coincided with normal distribution. While the moisture mainly distributed 9.3-12.1 g/100g, which was small and did not coincided with normal distribution (Fig. 2c). The crude protein, falling number, and flour yield coincided with normal distribution (Fig. 2c, d, and e).

3.2 Effects of grain characteristics on flour yield

The results of SEM were shown in Fig. 3 and Table 2. The final model fitted well as demonstrated by the CFI (0.975). Our primary aims were to simulate flour yield by applying path analysis among the five focal variables, and to assess the effects of five wheat grain characteristics on those comparisons. Overall, results support the view that test weight and hardness index each contribute uniquely to the flour yield. Those contributions, however, were largely limited by subjective cognitions because the SEM was based on an a priori theoretical model (Kline, 2015).

The direct effects of crude protein on hardness index were only 0.12 (Fig. 3). Comparing to the effects of test weight, exogenous factors (moisture content, falling number, and crude protein) had less effects on hardness index. The correlation factors of endosperm (moisture content, falling number, and crude protein) had no significant direct effect on flour yield, and the direct effects were only 0.03, -0.02, and -0.04, respectively (Fig. 3). But the total effects were 0.00, 0.10, and -0.11, respectively. And the maximum moisture content was only 13.7%. Test weight and hardness index had significant effect on flour yield, and the total effects were 0.313 and 0.432, respectively.

The significant direct effects on test weight were only -0.06, 0.28, and -0.24, respectively (Fig. 3). Moisture content, falling number, and crude protein were the compositions or could

change the construction of grain, and the influence on flour yield was more indirect effects by the test weight.

3.3 Regressive equation

Test weight and hardness index had the most important influence on flour yield, and the moisture content, falling number and crude protein had no significant direct effects on flour yield (Fig. 3). And so, test weight and hardness index were used to evaluate flour yield. The test weight represented the endosperm content of grain, which determined potential flour yield. And the hardness index represented the ease or complexity, which determined actual proportion of flour yield. The multiplicative effect rather than multiple linear regression was more suitable for the simulation of flour yield by the test weight and hardness index (Eq.3), and the R was 0.68.

$$\text{Flour yield} = 13.528 \times (\text{Test weight})^{0.179} \times (\text{Hardness index})^{0.104} \quad (3)$$

At the same time, about 617 samples in Northern part of Huang-huai Region were used to evaluate flour yield, which made the regressive equation had wider range of application. The regressive equation came from the statistical data. To improve its credibility, the observed data were used to verify the regressive equation. The observed and simulated flour yield evenly distributed around the 1:1 line (Fig. 4). The RMSE was 1.15 g/100g. The RRMSE was 0.018 which was less than 0.1. And so, the simulated result was excellent.

3. DISCUSSION

SEM was used to look for the most important wheat grain characteristics in Northern part of Huang-huai Region for flour yield, rather than all the wheat grain characteristics. And that can aid in the understanding and analysis the major factors of flour yield to quantify flour yield. The most important wheat grain characteristics were used to simulate flour yield. The regressive equation was based on theory instead of simple multiple linear regression. The

regressive equation was verified by field experiment in Yangling, which made the reliability of regressive equation was higher.

The larger CV of falling number was because the falling number was more effected by the precipitation during harvest period. Hagberg(Hagberg, 1960) developed the falling number to simply and rapidly determine α -amylase activity. a low falling number in wheat grain means high α -amylase, which causes poorer wheat quality(Edwards, 2010). And α -amylase usually occurs at harvest time when germination is initiated because of precipitation(Mares et al., 1986). While the precipitation during harvest period is a random occurrence, and has little effects by geographical regions. Classification on regions based on wheat quality in China cannot reflect the change of falling number very well. Test weight, hardness index, moisture content, and crude protein were affected by genotype and environment. The coefficients of variation of test weight, hardness index, moisture content, and crude protein were relatively small. Even though in a wheat quality region, the span of grain characteristics was still very large. The cultivars in Northern part of Huang-huai Region were white-hard-strong wheat. But with the effect of environment, the minimum hardness index was only 37, which was up to the standard of soft wheat. And the minimum crude protein was only 9.54 g/100g, also almost belonged to weak wheat. The mean values essentially belonged to white-hard-strong wheat.

The hardness index and test weight were large and didn't coincided with normal distribution. The cultivars were winter durum wheat, so the hardness index was large(Vignaux et al., 2005). The moisture was small. Thea was because the moisture content could be changed by artificial drying processes, and the lower moisture content was beneficial to the storage quality(Kalkan and Kara, 2011).

The combined effect of starch granule type and puroindoline content could determine 68% of the variation in flour yield (Edwards, 2010). But Topin, et al (Topin, et al, 2009) reported that the milling process was dominated by endosperm cohesion rather than the composition of

endosperm. The effects of moisture content, falling number, and crude protein on flour yield were more the indirect effects by test weight and hardness index. Moisture content had active influence on flour yield. Fang and Campbell et al (Campbell et al., 2007) recognized that the best moisture content for flour yield was 16-16.5%. And the maximum moisture content was only 13.7%. The larger moisture content shortened tempering time, and was beneficial to the flour yield. While falling number had active effect on flour yield. A low falling number meant high α -amylase, and a high α -amylase meant a high germination index which was harmful to the flour yield(Loshin, 2013). The high crude protein leaded to the lower density of endosperm in the grain, and that also reduced flour yield. Edwards(Edwards, 2010) recommend that protein content resulted flour was lower at lower extraction rates; however, the flour has greater strength.

The results were also like Haddad that test weight and hardness index appeared to be essential factors in wheat milling behaviour also important to the food processing industries(Haddad et al., 2001). The determinant of flour yield is the proportion of endosperm to grain which was 82-86%, and the proportion was correlative with test weight(Stenvert, 1972). Yan, et al(Yan et al., 2003) found that test weight has significant effect on flour yield in similar cultivar and environment. But Harris(Harris and Waldron, 1946) study results showed that no significant differences between test weight and flour yield were found in 659 samples of hard red spring wheat, and solely test weight to predict accurately milling was danger. Moisture content, falling number, and crude protein had no significant direct effect on flour yield, but they had significant direct effect on test weight.

Hardness index significantly correlates with wheat flour yield, and correlation hardness index with wheat vitreousness has been found out(Koeksal et al., 1993). The hardness was determined by the binding force between starch granules and storage protein(Simmonds et al., 1973). Vitreousness is affected by the starch granules of different sizes which are coated by a

protein matrix created predominantly by gluten proteins(Morris et al., 1999). But Zhou, et al.(Zhou et al., 2002) recognized that cutin rate and the composition of cutin were marked positive correlated with hardness. The less effects of exogenous on hardness index was because the vitreousness and cutin had more effects on hardness index. The construction rather than composition had more effects on hardness index, crude protein still had significant effects on hardness index. But they were difficult to determine. The crude protein had the greatest effect (0.12) on hardness index. Greenaway(Greenaway et al., 1969) reported that protein played significant roles, and affected endosperm texture.

The flour yield was difficult to simulate, but which was vital to the economic benefits of flour mills(Dobraszczyk et al., 2002). The multiple linear regression of glutenin subunit compositions for flour yield showed that the R of simulated result was only 0.45(Bi and Long, 1996). Though the R of this study was still only 0.68, the simulation result was better than most of other results(Bi and Long, 1996; Edwards, 2010; Flores et al., 1991; Loza-Garay and Flores, 2003; Mog, 2011).The flour yield for a given cultivar would be different, if it was under different managements or in different sites. Even the grains in different parts of a same spike(Campbell et al., 2007).

4. CONCLUSION

This study with large samples data analysed direct and indirect influences of grain characteristics on flour yield by SEM and quantified the relationship between grain characteristics and flour yield.

(1) The CV of grain characteristics was low and distributed rather closely. The hardness index and test weight of winter durum wheat was larger, and the moisture was lower.

(2) Test weight had the most significantly effects on flour yield, followed by the hardness index. The effects of moisture content, falling number, and crude protein on flour yield were more the indirect effects by test weight and hardness index.

(3) Grain characteristics could excellently estimate flour yield, and which could determine 68% of the variation in flour yield. The RRMSE of regressive equation was 0.018, and the simulation result was excellent.

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Fig. 1 The sampling sites of Northern part of Huang-huai Region in China. There were total 104 sites and 69 cultivars from 2008 to 2016.

Fig. 2 Probability distributions of the winter durum wheat grain characteristics

Fig. 3. Fitted observed variable model. Comparative fit indexes are displayed for significant ($p < 0.05$) paths. Path width is proportional to the magnitude of the comparative fit index. Imaginary line represents indirect effect, and full line represents direct effect. Significance level: $*p < 0.001$; $**p < 0.01$; $*p < 0.05$.**

Fig. 4. Simulated and observed flour yield in 2015 and 2016 under different nitrogen and water stresses to validate regressive equation. The dotted line is the 1:1 line.

Table 1 Summary of the 617 samples collected from the Northern part of Huang-huai Region from 2008 to 2016.

Variables	Minimum	Maximum	Mean value	Coefficient of variation
Hardness index (dimensionless)	37	73.5	62.27	9.84 %
Test weight (g/L)	730	847	801.82	2.24 %
Moisture content (g/100g)	8.2	13.7	10.69	7.62 %
Crude protein (g/100g)	9.54	17.51	14.04	8.03 %
Falling number (s)	80	502	354.54	16.68 %
Flour yield (g/100g)	44.1	77.1	68.90	4.30 %

Table 2 Direct, indirect, and total effects of grain characteristics on flour yield.

Variables	Direct effect	Indirect effect	Total effect
Hardness index	0.313	-	0.313
Test weight	0.432	-	0.432
Moisture content	0.028	-0.028	0.000
Falling number	-0.021	0.121	0.101
Crude protein	-0.045	-0.065	-0.110