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ABSTRACT

In bread-making, various quality criteria describe dough behaviour, but their determinants and relationship to flour composition remain unclear. This study examined 282 wheat bread flour samples representative of French wheat-growing conditions that were used to address this issue using statistical modelling. The quality criteria analysed include alveograph variables—elasticity index (Ie), baking strength (W), tenacity (P), extensibility (L), and the tenacity-to-extensibility ratio (P/L)—as well as quantitative variables from the bread-making test, such as bread volume (BV) and dough elongation at shaping (DE). An in-depth biochemical characterisation of the flour samples was performed, measuring proteins, starch, lipids and arabinoxylans. A model selection approach based on the Bayesian Information Criterion (BIC) and the Variance Inflation Factor (VIF) was applied to identify the key determinants of these quality criteria, integrating the influence of composition variables on water absorption. Results indicate that farinograph water absorption significantly influences W and P, but not Ie and DE, which are more strongly determined by gluten-related variables. Notably, arabinoxylans impact all quality criteria, while lipids significantly affect W and DE. Finally, our results revealed a strong dependency between Ie and dough elongation under French bread-making conditions.

1. Introduction

Crop production is undergoing major transitions due to climate change and the increasing demand for organic, local and clean-label products (Feil and Stamp, 1993; Le Gouis et al., 2020). Additionally, the European baking industry must adapt to strict production constraints that limit the use of additives to mitigate the impact of flour variability. These changes further strengthen the role played by wheat flour quality in the baking industry, underlining the need for a detailed understanding of wheat quality traits, in particular, the grain and flour composition characteristics involved in dough behaviour during processing.

In many countries, standard tests are routinely used to assess wheat quality after harvest. Protein content is a primary factor of bread wheat quality worldwide, alongside other key quality criteria such as: the Hagberg Falling Number (HFN), which indicates potential sprout damage; grain hardness, which is related to the flour's damaged starch content; and specific weight, which is an indication of flour milling yield. In addition, functional protein properties are often evaluated through wet gluten, dry gluten and gluten index measurements. **Technological tests** are based on instruments such as the Farinograph© (Brabender) and the Alveograph© (Chopin), which are widely used to assess flour functionality. The farinograph provides the widely used flour Water Absorption (WA) value, while the alveograph performs a bubble inflation test of the dough (Dobraszczyk and Robert, 1994) to assess rheological properties such as extensibility (L), tenacity (P), baking strength (W) and elasticity index (Ie). These measurements are used in the bakery sector to anticipate dough performance in terms of production and support decision-making regarding the suitability of the flour for industrial processing. In addition to the technological tests, standardised baking tests such as the standard NF V03-716 in France are important references since they reproduce realistic bread-making under controlled conditions. The French standard includes subjective scoring with objective bread quality descriptors such as Bread Volume (BV) and Dough Elongation during shaping (DE). BV is traditionally associated

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with wheat baking quality (Ziegler et al., 2025), whereas DE has been identified as a valuable descriptor of dough behaviour in related works and should also be associated with baking quality (Munch et al., 2024). Since baking tests are particularly resource-consuming, it is essential to identify wheat quality characteristics that can predict baking quality (Ziegler et al., 2025). Many studies have attempted to predict bread quality from compositional and technological variables, but accurately predicting BV has proven to be a challenge (Selga et al., 2024) unless the baking test is adapted for this purpose (Ziegler et al., 2025). Like BV, DE is measured in real bread-making conditions (NF V03-716) and serves as a direct bread quality indicator, distinguishing it from technological test measurements. It is therefore interesting to study DE and to assess the influence of both major and minor components on this property.

Several publications report relationships between grain and flour composition characteristics and properties measured with technological tests and baking tests. The effect of protein characteristics on alveograph measurements is one of the aspects that has been extensively studied. It has been shown across several studies that protein content alone exhibits moderate correlations with W ($R = 0.44–0.67$) (Popa et al., 2009; Rasper et al., 1986; Gaines et al., 2006). Protein composition—particularly the proportion of high molecular weight glutenin subunits— significantly influences W and Ie, and the wet ($r = 0.77$) and dry gluten contents ($r = 0.80$) influence Ie, underlining the importance of gluten network quality in dough performance (Yousaf et al., 2019; Guzmán et al., 2022). Other works reported that flours with high levels of damaged starch presented high P values with reduced bubble expansion, mirrored by low L and W values (Dexter et al., 1994; Preston et al., 1987).

However, the role of **minor flour components**, particularly **lipids** and **arabinoxylans**, remains underexplored despite their significant contribution to bread quality (Marion and Saulnier, 2020). In particular, their effects on dough rheology and baking quality are not well characterised. In Selga et al. (2024), the water-unextractable arabinoxylan content (WU-AX) was included in a prediction model of the bread loaf volume, along with the alveograph parameters and the damaged starch. In a previous work, we showed that the specific viscosity of water-extractable arabinoxylans (SV.AX) significantly contributed to the prediction of WA in combination with protein and damaged starch-related variables (Rezette et al., 2025). This suggests that minor components can influence dough behaviour via their impact on WA.

In this work, we evaluated the hypothesis that flour composition, particularly minor components, can influence dough rheology and baking quality, in addition to flour water absorption, using a model selection method. A dataset of 282 flour samples of wheats harvested in 2020, 2021 and 2022 was used in combination with data concerning flour composition (proteins, starch, lipids and arabinoxylans), alveograph measurements (W, P, L, P/L, Ie) and bread quality indicators (DE and BV). With the aim to identify key flour components for the prediction of alveograph and baking quality variables, multiple regression models were generated and screened using the Bayesian Information Criterion (BIC) score and the Variance Inflation Factor (VIF) so as to select the most robust, interpretable predictive models. The effect of flour water absorption was computed from the flour composition using an existing model in order to distinguish this effect from the other effects of the flour components. Finally, the modelling of DE is being further developed for the purpose of reducing the systematic use of baking tests.

2. Materials and methods

2.1. Plant material

A total of 290 grain samples harvested over three years (2020, 2021 and 2022), corresponding to 99 cultivars of *T. aestivum* wheat grown in 39 locations across France, were supplied by Arvalis, Limagrain and Axiane Meunerie. Each sample was assigned an expected usage by wheat breeders based on its genotype. Among the 290 wheat samples, 191 were designated for bread-making application (WBM), 17 for biscuit application (WB), 63 as improvers for bread-making (WI), and 19 for other uses (WOU).

The grains were milled into white flour with an experimental mill (MCKA, Bülher, Switzerland) in batches of 10 kg. Extraction rates ranged from 60.6 % up to 78.1 %, with an average value of 71.8 % (Munch et al., 2025). Flours were then stored for 20 days at room temperature and then frozen at −20 °C until analysis.

2.2. Flour and dough characterisation

A wide range of grain, flour and dough analyses were performed on the collection to characterise the wheat quality. All data are available on a data paper (Munch et al., 2025).

The technological variables consisted of the flour water absorption (WA) measured by the Mixolab (Chopin Technologies, France; ISO 5530–1:1997), alveograph parameter tenacity (P), extensibility (L), tenacity-to-extensibility ratio (P/L), baking strength (W) and elasticity index (Ie) (Chopin Technologies, France; NF EN ISO 27971). The bread quality indicators included bread volume (BV) and dough elongation at shaping (DE), both determined during the standardised baking test (NF V03-716). BV was quantitatively measured, while DE was traditionally evaluated using a seven-level rating grid. In this study, DE—corresponding to the dough's length after shaping—was also measured manually with a ruler and expressed in centimetres. This study focused on analysing the quantitative data from the baking test, whereas the sensory data was analysed elsewhere (Munch et al., 2024). Classical flour characterisation was carried out and included the Damaged Starch (SD) value measured by SDmatic (Chopin, France, ISO 17715:2015).

Advanced characterisation of flour composition was also carried out according to methods described in detail in Rezette et al. (2025) and in Munch et al. (2025). In addition to SD, the composition variables for polysaccharide characterisation included total arabinoxylan content (TOTAX), water-extractable arabinoxylan content (WEAX), the arabinose-to-xylose ratio from total arabinoxylans (A/X.TOT), the arabinose-to-xylose ratio from water-extractable arabinoxylans (A/X.WE), and soluble starch (SS). Polysaccharides in the flours and their water extract were hydrolysed into monomers by acid hydrolysis, and the resulting individual neutral sugars were quantified by gas-liquid chromatography after conversion to alditol acetate, as previously described in Rezette et al. (2025). For each variable, the average of three replicates was determined per sample. The specific viscosity from water-extractable arabinoxylans (SV.AX) and the intrinsic viscosity from water-extractable arabinoxylans (IV.AX), representing the physico-chemical traits of the soluble fraction, were analysed as described by Rezette et al. (2025) using a high-performance size-exclusion chromatography (HPSEC) system (OMNISEC RESOLVE-REVEAL; Malvern Panalytical, Malvern, UK), with a Viscotek AGuard precolumn (50 × 6 mm) and a Viscotek A4000 column (300 × 8 mm) (Malvern Panalytical, Malvern, UK), maintained at 35 °C, and eluted with 50 mM sodium nitrate at a flow rate of 0.7 mL/min. To ensure repeatability of HPSEC measurements, the same commercial flour sample was repeatedly analysed (4–5 times) throughout the analytical sequence, confirming a coefficient of variation (CV) below 5 %.

Flour protein composition was determined from the high-performance size exclusion chromatography (HPLC Alliance, Waters) analysis of two sequential extractions, as described in Morel et al. (2000) and Rezette et al. (2025). The chromatogram of the first extract was divided into five fractions of decreasing molecular weight ranges. Fraction F1 and F2 were assigned to the soluble glutenin content (GluS), whereas F3 and F4 were assigned to gamma, beta and alpha gliadin content (Gli). The total area of the second extract chromatogram made it possible to obtain the Insoluble glutenin content (GluI). Total protein content (Prot) was also calculated. Due to the large number of samples and the time required for analysis, single analyses were performed. To ensure repeatability and reliability, 10 samples picked at random were repeatedly analysed 3 to 4 times, confirming that the measurements had a coefficient of variation (CV) of less than 5 %.

Finally, for lipid characterisation, total palmitic acid C16 content (C16.TOT), total stearic acid C18 content (C18.TOT), total vaccenic acid C18:1n-7 content (C181n7.TOT), total oleic acid C18:1n-9 content (C181n9.TOT), total linoleic acid C18:2n-6 content (C182n6.TOT) and total alpha-linolenic acid C18:3n-3 content (C183n3.TOT) were measured after acid hydrolysis and transmethylation with quantification of fatty acids by GLC based on the method used In Welch (1977). For each variable, the average of three replicates was determined per sample.

All contents are expressed in g per 100 g of flour (wb). Units are given in Supplementary Data S1.

2.3. Data treatment for alveograph variables and quality indicator prediction

Out of the initial 290 wheat samples, eight were excluded from the modelling due to missing data, resulting in a total of 282 samples for the analysis.

For the purpose of model construction, alveograph measurements are categorised as technological variables, DE and BV are designated as quality indicators, and composition measurements are referred to as composition variables. Our approach to revealing significant relationships between technological variables and quality indicators, on the one hand, and composition variables, on the other, involves selecting regression models. In these models, composition variables serve as explanatory variables and technological variables/quality indicators are treated as response variables.

2.3.1. Analysis of linear correlations between the variables

Linear correlations (Pearson coefficient) between all the variables were analysed by means of a clustermap. A clustermap is a correlation matrix whose columns are ordered according to the results of a hierarchical clustering technique. The hierarchical clustering reorders the variables by similar correlations according to Euclidean distance and average linkage aggregation. The generated hierarchical clustering tree, or dendrogram, was added at the top of the matrix. The clustermaps were produced using the *heatmap.2* function from the R package, *gplots*, under R v4.1.3.

2.3.2. Including water absorption (WA) as a latent variable

Flour WA exerts an effect on dough and bread properties that can be accurately predicted from composition variables, as shown in a previous study (Rezette et al., 2025). However, it is necessary to distinguish this effect from other ways in which composition variables impact dough and bread properties. For example, flour composition directly affects gluten network properties in addition to its influence on WA.

To isolate the effects of flour composition unrelated to WA, WA was introduced as a latent variable in the regression models. WA was computed from composition variables using a four-variable regression model presented in a previous work (Rezette et al. (2025), which analyses an extract of the database used in the present work. This model generates WAM, a simulated WA variable, from four composition variables: Prot, SS, SD and SV-AX. In Rezette et al. (2025), these four variables were included in the regression model that offered the best trade-off between predictive accuracy of WA and the number of explanatory variables. Thus, WAM is computed using this model and used as an explanatory variable instead of WA. While standardised coefficients were used in Rezette et al. (2025), they have been converted here into real values to match the units of the variables, resulting in the following model:

$$WAM = 0.99*Prot + 0.96*SS + 0.27*SD + 5.8*10^{-3}*SV.AX + 36.3 \quad (1)$$

where Prot and SS are in g/100 g, SD is in UCDc and SV.AX is in mV·mL.

2.3.3. Model selection

To analyse the effect of composition on technological variables and bread quality indicators, linear regression models were selected following the approach described in Rezette et al. (2025). Each regression model simulates a technological variable or a bread quality indicator (response variable) from flour composition variables (explanatory variables). The explanatory variables are standardised to analyse their relative effects. The model selection procedure aims at selecting the regression model that obtains the best trade-off between a minimum number of explanatory variables and the best predictive performance. This procedure relies on two statistics, the Bayesian Information Criterion (BIC) that is used to rank models based on the residuals and on the number of variables (the BIC penalises a growing number of variables, contrary, for example, to what the R^2 would do), and the Variance Inflation Factor (VIF) that is used to exclude models with highly correlated explanatory variables. A VIF value greater than five is generally considered to be an indicator of high multicollinearity. Therefore, all models presenting a value of above five were excluded from the selection. In addition, regression models whose p-values coefficients were below 0.001 were given priority for selection so as to ensure that the interpretation of the effects was supported a by sufficient level of significance. For each candidate model, a BIC score is computed as the difference between the BIC of the model and the BIC of a control model, which is the mean value of the response variable. The lower the BIC value is, the higher the predictive performance of the model will be; therefore, the BIC score of a model is negative.

The predictive performance of each candidate model is assessed with a repeated K-fold cross validation according to the procedure described in Rezette et al. (2025). A cross-validation R^2, denoted R^2_{CV}, is computed in addition to the BIC score and the VIF. The selected model that achieves the best compromise between performance and interpretability is referred to as the Model of Interest (MOI).

In practice, models with the highest predictive performances tend to be challenging to interpret due to an excessive number of variables (risk of overfitting). Conversely, models with lower predictive performances generally include the variables with the strongest effects, making them more robust and easier to interpret. In that respect, the MOI is chosen to favour interpretability and robustness over pure predictive performance.

Statistical analyses were performed with R v4.1.3. The Bayesian Information Criterion (BIC) test was assessed using the *regsubset* function from the R package, *leap*, and the Variance Inflection Factor (VIF) was calculated using the *vif* function from the R package, *car*.

3. Results

3.1. Sampling variability

The range of values for composition variables is summarized in Supplementary Data S1, while the values for technological variables and bread quality indicators are presented in Table 1.

The min-max ranges for tenacity P (22–143 mm) and for the tenacity-to-extensibility P/L ratio (0.13–2.74) are lower and narrower than the ones reported in Yousaf et al. (2019) (54–218 mm and 0.55–5.45, respectively, for 36 samples), but are consistent with the ranges obtained by Jødal and Larsen (2021) (26–110 mm for P and 0.15–2.28 for P/L), on 532 alveograph curves from different flour qualities and/or dough compositions. The range for extensibility L (41–181 mm) is close to the values reported in Yousaf et al. (2019) (34–190 mm) and in Jødal and Larsen (2021) (29–207 mm). Finally, the min-max ranges for the elasticity index Ie (20–73 %) and the baking strength W (67–546 0.10^{-4}J) are rather large compared to those reported in Jødal and Larsen (2021) (31.1–61.5 % and 62-352.10^{-4}J, respectively) and in Yousaf

Table 1
Descriptive statistics of the technological variables (WA, P, L, P/L, Ie, W) and quality indicators (DE, BV), for the 282 wheat samples.

Unit	WA	P	L	P/L	Ie	W	DE	BV
	%	mm	mm	/	%	10^{-4} J	cm	cm^3
Min-Max	50.3–63.9	22–143	41–181	0.13–2.75	25–73	67–546	20–44	940–2080
Mean	56.2	74	99	0.84	54	234	30	1640
CV (%)	4.6	28.5	28.5	50.1	15.8	37.6	12.8	13.8

WA: Water Absorption; P: Tenacity, L: Extensibility, P/L: Tenacity to extensibility ratio P/L, W: Baking strength, Ie: Elasticity index, DE: Dough Elongation at shaping; BV: Bread Volume. CV: Coefficient of Variation.

et al. (2019) (42–77 and 93–437 0.10^{-4}J, respectively). The CV of Ie (15.8 %) is much lower than that of P/L (50 %), as observed by Kitissou (1995). The CV of Ie is also much lower than that of P and L (28.5 % for both) or W (37.8 %), but in the same range as DE (12.8 %). To our knowledge, values for DE have never been reported in the related literature. The range for WA (50.3–63.9 %) is lower compared with the one reported by Sapirstein et al. (2018) (53.9–65.5 % for 78 samples). Given that P is generally affected by the water absorption (Preston et al., 1987) the low values of P in our dataset are consistent with the rather low values of WA. The differences in the range of technological and compositional parameters observed between our study and those reported in the literature are relatively minor and typical for this type of investigation, primarily reflecting variations in the genetic background and environmental growing conditions of the wheat samples analysed.

As previously indicated, wheat samples are classified according to their intended use by wheat breeders. Fig. 1 shows the distribution of the 282 samples on a PCA map based on the technological variables and quality indicators presented in Table 1. Wheats for biscuit applications (WB) typically have lower WA, P, W and P/L values and higher DE values. In contrast, "improver" wheat (WI) generally has lower DE values and higher W, IE and WA values. Among these technological variables and quality indicators, L is the least effective in distinguishing between wheat sample types.

3.2. Results: wheat determinants of dough behaviour

3.2.1. Exploring correlations in the dataset

A clustermap obtained from the correlation matrix with all variables of the dataset is provided in Supplementary Fig. S2. Given the size of the dataset, even a weak correlation of $r = 0.20$ is highly significant (p-value <0.001). Three clusters were identified (a, b and c; see Supplementary Fig. S2).

The first cluster (a) includes P, W and Ie from the alveograph, along with DE, WA and WAM, SS and protein-related variables. WA and WAM show a strong correlation ($r = 0.89$), confirming that WAM is a reliable model for WA. WA correlates with P and W ($r = 0.76$ and 0.75, respectively), in agreement with the literature (Jødal and Larsen, 2021; Konopka et al., 2004; Preston et al., 1987). Additionally, P is correlate with damaged starch variables, SS and SD, confirming previous observations (Dexter et al., 1994), which can be explained by its relationship with WA. Protein-related variables—protein content (Prot), gliadin content (Gli) and insoluble glutenin content (GluI)—are strongly correlated with Ie and W, WA, WAM and DE, and to a lesser extent with P. These overall correlations between protein content and alveograph variables are consistent with previous studies (Baudouin, 2023; Jødal and Larsen, 2021; Kitissou, 1995; Konopka et al., 2004; Popa et al., 2009; Rasper et al., 1986; Yousaf et al., 2019). Interestingly, dough elongation (DE) is strongly correlated with Ie ($r = -0.86$) and W ($r = 0.77$). Additionally, although L is expected to represent dough extensibility during mixing, it shows no clear relationship with dough

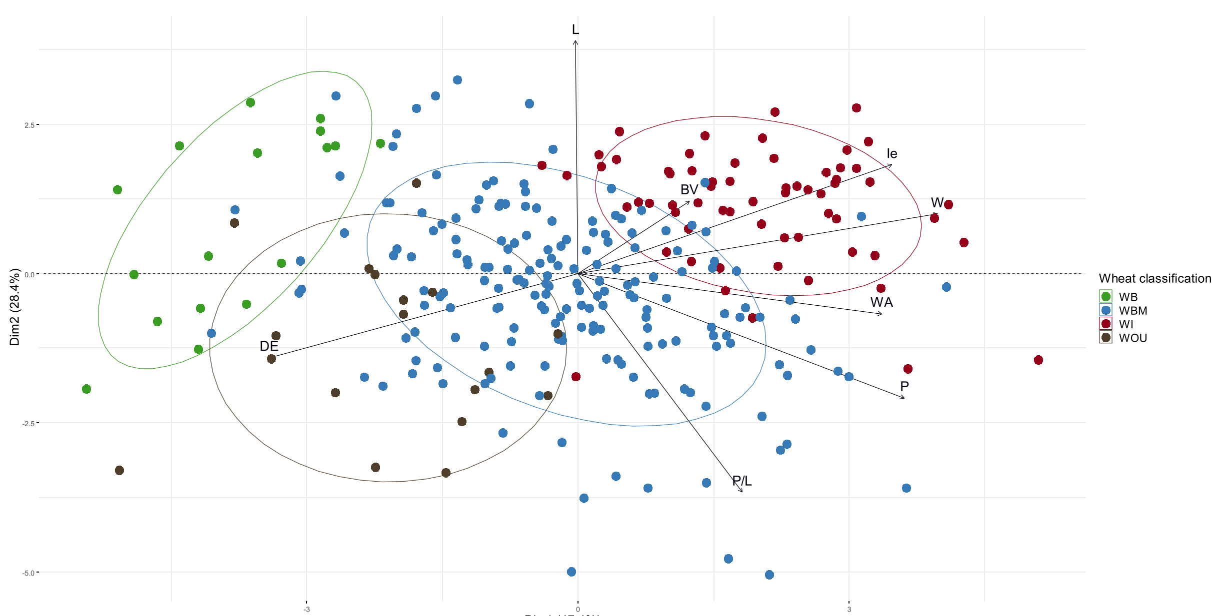

Fig. 1. First two dimensions of the Principal Component Analysis (PCA) of six technological variables (P, L, P/L, W, Ie, WA) and two bread quality indicators (DE, BV) for 282 wheat samples. The legend indicates the classification of the wheats studied according to their intended end-uses.
WB: Wheat for Biscuit applications; WBM: Wheat for Bread-Making; WI: Improver Wheat; WOU: Wheat for Other Uses;
WA: Water Absorption; P: Tenacity; L: Extensibility; P/L: Tenacity-to-extensibility ratio; W: Baking strength; Ie: Elasticity index; DE: Dough Elongation at shaping; BV: Bread Volume.

elongation at shaping (DE), as indicated by a weak negative correlation ($r = -0.2$; see Supplementary Fig. S2).

The second cluster (b) includes three subgroups of correlated variables comprising lipid-related variables, with the exception of C18.TOT, two arabinoxylan-related variables, A/X.WE and A/X.TOT, as well as L and GluS. Apart from a correlation with GluS ($r = 0.60$), L appears to be less closely related to composition variables compared to other alveograph variables.

The third cluster (c) encompasses variables that are generally less correlated with the other variables, e.g., BV, AXTOT, or which present distinctive correlation profiles compared to cluster (a) and (b), e.g., P/L, IV.AX, WEAX, SV.AX.

Concerning arabinoxylans, no significant correlations were observed with the technological variables or quality indicators investigated. However, lipids, particularly the total linoleic acid C18:2n-6 content (C182n6.TOT), are correlated with both W ($r = 0.52$ with C18:2n-6.TOT) and Ie ($r = 0.53$ with C18:2n-6.TOT). Unfortunately, this group of variables is also correlated with Prot ($r = 0.61$ with C18:2n-6.TOT), which prevents the analysis of their independent effects on dough behaviour separately from proteins.

3.2.2. *Identifying determinants of dough behaviour with multiple linear regression*

Multiple linear regression was used to identify the main compositional determinants of dough behaviour variables, Ie, W, P and DE, from a set of wheat flour components that included proteins (Prot, GluI, GluS, Gli), damaged starch (SD, SS), arabinoxylans (WEAX, AXTOT, A/X.WE, A/X.TOT, SV.AX, IV.AX), lipids (C16.TOT, C18.TOT, C181n1n7.TOT, C181n9.TOT, C182n6.TOT, C183n3.TOT).

As explained in Section 2.3, flour water absorption (WA) is not directly used as an explanatory variable. Instead, it is included as a latent variable, denoted WAM, which is computed using Eq. (1). WAM captures the combined influence of Prot, SS, SD, and SV.AX on water absorption.

The model selection process ranks candidate models based on **Bayesian Information Criterion (BIC)** score values. Models with **Variance Inflation Factor (VIF) scores above five** are excluded to avoid multicollinearity issues (see Supplementary Fig. S3).

Table 2 summarizes the selected models for each dough variable. It presents the standardised regression coefficients, indicating the relative contribution of each explanatory variable. The Model of Interest (MOI) that presents the best trade-off between prediction performance and interpretability is highlighted in grey.

Table 2

Summary of models selected on the basis of Bayesian Information Criterion (BIC) and Variance Inflection Factor (VIF) tests for A) Ie, B) W, C) P and D) DE, denoted respectively M-Ie, M-W, M-P, M-DE.

A)	Proteins variables	Damaged starch variables		Arabinoxylans variable	Statistical metric values		
	GluI	SD	SS	A/X.TOT	n[a]	R^2cv	BIC score
M-Ie$_{GluI}$	0.87				1	0.74	−379.7
M-Ie$_1$	0.88	−0.20			2	0.78	−423.1
M-Ie$_2$	0.85	−0.29	0.17		3	0.80	−444.3
M-Ie$_3$	0.83	−0.25	0.14	0.10	4	0.81	−451.6

B)	Proteins variables		Damage starch variables		Arabinoxylans variables			Lipids variables			Predicted variable	Statistical metric values		
	GluI	Gli	SD	SS	IV.AX	SV.AX	WEAX	C18.TOT	C181n9.TOT	C182n6.TOT	WAM	n[a]	R^2cv	BIC score
M-W$_{GluI}$	0.85											1	0.72	−353.3
M-W$_1$	0.63										0.34	2	0.78	−420.3
M-W$_2$	0.54	*0.13*			*−0.11*	*0.11*		*−0.09*	*−0.10*	*0.09*	0.31	8	0.81	−436.8
M-W$_3$	0.64							−0.14			0.38	3	0.80	−439.1
M-W$_4$	0.63	0.29	0.15	*0.09*	*−0.11*	0.22		−0.14				7	0.81	−439.8
M-W$_5$	0.55	*0.13*			*−0.08*	*0.10*		−0.13			0.32	6	0.81	−442.3
M-W$_6$	0.57	*0.13*						*−0.12*			0.33	4	0.81	−444.1
M-W$_7$	0.56	0.18					*0.08*	−0.13			0.29	5	0.81	−445.8

C)	Proteins variable	Arabinoxylans variables	Predicted variable	Statistical metric values		
	GluS	AXTOT	WAM	n[a]	R^2cv	BIC score
M-P$_{WAM}$			0.73	1	0.53	−206.8
M-P$_1$	−0.34		0.86	2	0.63	−267.2
M-P$_2$	−0.33	0.13	0.85	3	0.64	−274.1

D)	Proteins variables		Arabinoxylans variables		Lipids variables		Statistical metric values		
	GluI	GluS	IV.AX	WEAX	C18.TOT	C181n9.TOT	n[a]	R^2cv	BIC score
M-DE$_{GluI}$	−0.79						1	0.62	−263.6
M-DE$_1$	−0.85				0.20		2	0.65	−287.9
M-DE$_2$	−0.82				0.22	−0.13	3	0.66	−294.5
M-DE$_3$	−0.86	0.16	0.17		0.18		4	0.67	−301.3
M-DE$_4$	−0.84	0.18	0.16	*−0.07*	0.22	−0.13	6	0.69	−306.0
M-DE$_5$	−0.85	0.18	0.14		0.21	−0.13	5	0.68	−307.6

Variables were standardised for each linear regression model and their corresponding coefficients are indicated. The models are ranked in ascending order of predictive performance, the ranking being indicated in the form of indices, except for the univariate model, which mentions the name of the variable. Terms in the models considered not significant (p-value ≥0.001) are in italic. Grey-shaded model is the Model Of Interest (MOI). The BIC score indicated is the difference between the BIC from the model and the BIC from the control i.e the mean value of the response variable. R^2_{CV}: cross-validation coefficient of determination.

GluI: Insoluble Glutenin content, GluS: Soluble Glutenin Content; Gli Gliadin content; SD: Damaged starch measured by iodine absorption; SS: Soluble Starch; A/X.TOT: Arabinose on Xylose ratio from Total Arabinoxylan content; IV.AX: Intrinsic viscosity of arabinoxylans; SV.AX: Specific viscosity of arabinoxylans; WEAX: Water-Extractable Arabinoxylans; AXTOT: Total Arabinoxylan content; C18.TOT: Total stearic acid C18 content; C181n9.TOT: Total oleic acid C18:1n-9 content; C182n6.TOT: Total linoleic acid C18:2n-6 content; WAM: Water Absorption simulated from total protein content, Soluble Starch, Damaged Starch and Specific Viscosity of Arabinoxylans; Ie: Elasticity Index; W: Baking Strength; P: Tenacity; DE: Dough Elongation at shaping.

[a] Number of variables included in the model.

The performances of the models for L and for P/L were particularly poor ($R^2_{CV} < 0.5$); they are provided in Supplementary Data S4. The performances of the models obtained for BV are anecdotal and data is therefore not reported. Table 2A, 2.B, 2.C and 2D report the best single-variable models in the first rows. GluI is the variable selected for Ie, W, P and DE, whereas it is WAM for P.

For Ie (Table 2A), the MOI is M-Ie_3, with a R^2_{CV} of 0.81. M-Ie_3 includes one variable related to proteins (GluI), two related to damaged starch (SD and SS), and one related to arabinoxylans (A/X.TOT). The amount of insoluble glutenin (GluI) remains the primary compositional characteristic impacting Ie, which confirms the observations reported by Baudouin (2023). Damaged starch tends to reduce Ie (coefficients of SD and SS have opposite signs, but SD has a much greater effect in the model than SS). This confirms the results of Kitissou (1995) who reported that excessive starch damage leads to a reduction in the dough's elastic strength.

The MOI of W (Table 2B) (M-W_3), with a R^2_{CV} of 0.80, is composed of GluI, C18.TOT and WAM. As for Ie, GluI is the most important variable for predicting W. According to M-W_4, the only model without WAM, damaged starch variables have a positive effect on W, along with Prot and SV.AX; this is captured by WAM in other models of the series.

The MOI of P (Table 2C) (M-P_2), which has a R^2_{CV} of 0.64, is composed of WAM, GluS and AXTOT. The relative effect of WAM is particularly strong. This agrees with the results reported in the literature (Álava et al., 2007; Preston et al., 1987).

The MOI of DE (Table 2D) (M-DE_5), with a R^2_{CV} of 0.68, is composed of five variables—GluI and GluS, C18.TOT and C181n9.TOT, and IV.AX—in order of importance.

4. Discussion

Fig. 2 summarizes the relationships represented by the MOI from Table 2 in the form of a causal graph.

4.1. Gluten/protein impact

The proteins generally associated with the gluten network, GluI and GluS, have a strong impact on the selected quality criteria of the dough. According to Kitissou (1995), Ie measures the resistance of dough to deformation, which reflects the internal bonding forces within the dough bubble membrane during alveograph inflation. In our study, we found that Ie is primarily influenced by the insoluble glutenin fraction (GluI), which corresponds to high molecular weight glutenin polymers known to significantly contribute to dough strength (MacRitchie, 2014). This result confirms that the specific aspects of protein composition, particularly the proportion of HMW glutenins, play a key role in determining dough elasticity.

Dough behaviour at the optimal water content for French bread-making tests was evaluated by measuring dough elongation at shaping (DE). Similar to Ie, DE is primarily influenced by GluI, but with an opposite effect. The modelling of DE appears to mirror that of Ie as both are described by the same protein-related variables. W is also explained by GluI, unlike P, which is mainly impacted by soluble glutenin (GluS). Among the other dough behaviour variables, only DE is slightly impacted by GluS.

4.2. Water absorption impact

Among all the alveograph output variables, P is highly dependent on WAM, while W shows a moderate dependency. Given that W and P

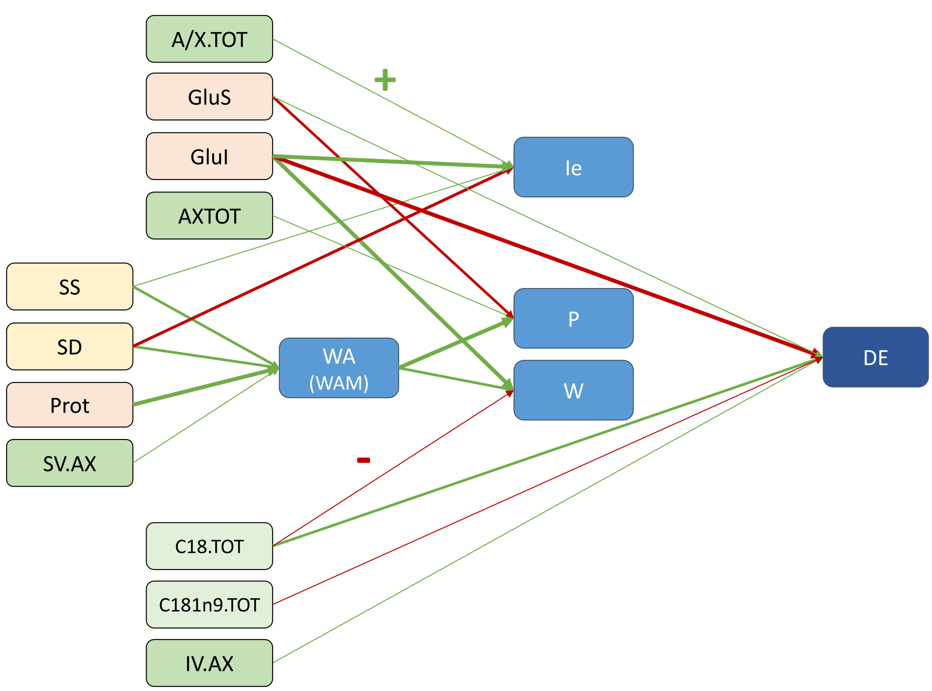

Fig. 2. Summary of flour composition effects on dough behaviour variables (Ie, P, W and DE), integrating their effects on WA via WAM (Predicted Water Absorption). Green and red arrows are for positive and negative effects, respectively. The greater the width of the arrow, the stronger the effect.
In light red, Prot: Protein content; GluI: Insoluble Glutenin content; GluS: Soluble Glutenin Content;
In yellow, SS: Soluble Starch; SD: Damaged starch measured by iodine absorption;
In dark green, AXTOT: Total arabinoxylan content; A/X.TOT: Arabinose-to-Xylose ratio from AXTOT; IV.AX: Intrinsic viscosity of arabinoxylans; SV.AX: Specific viscosity of arabinoxylans;
In light green, C18.TOT: Total stearic acid C18 content; C181n9.TOT Total oleic acid C18:1n-9 content;
In light blue, the technological variables, WA: Water Absorption/WAM: Predicted Water Absorption; Ie: Elasticity Index; W: Baking Strength; P: Tenacity;
In dark blue, the quality indicator DE: Dough Elongation at shaping.

reflect the dough consistency (Codina et al., 2012), it is not surprising that water absorption affects these two variables.

The contributions of Prot, SS, SD and SV.AX to flour water absorption are captured through WAM (see Eq. (1)). The impact of proteins and water absorption—resulting from increased levels of damaged starch and bran (arabinoxylans)—on P, has already been reported in the literature (Álava et al., 2007; Preston et al., 1987).

Alveograph measurements are performed at 50 % dough hydration (flour basis), which is generally below the optimal level for bread-making, as observed in our dataset. Under these conditions, a competition for water among the flour components is likely to occur, particularly during the initial mixing phase of bread-making. However, Ie does not appear to be significantly related to flour water absorption since WAM is not included in the candidate models (Table 2A). Substituting WAM with WA in the model selection process revealed no relationships between Ie and WA either (data not shown). This suggests that Ie remains stable across different hydration levels, unlike P and W. This finding implies that, under alveograph conditions, gluten is adequately hydrated to contribute to the dough's elastic properties, and that water also acts as a lubricant, with its viscosity varying depending on the levels of WEAX (Rezette et al., 2025), thereby affecting P and W. The competition for water is expected to become less pronounced—or even negligible—at optimal hydration levels once the dough reaches a homogeneous state, such as during dough shaping. Like Ie, DE is not impacted by WAM (or by WA).

4.3. Impact of non-protein components beyond WA

Soluble starch (SS) has been proposed as a marker of the damaged starch, complementing SD. Both SS and SD were found to be useful in modelling WA (Eq. (1)) (Rezette et al., 2025). The modelling of Ie shows that SS and SD also substantially contribute to Ie, but with opposing effects (see Table 2A). This suggests an effect of damaged starch on Ie not related to WA, the nature of which remains to be determined.

The present work indicates that total arabinoxylan content (AXTOT) exerts a small but significant effect on P, in addition to the influence of specific viscosity from water-extractable arabinoxylans (SV.AX) via WAM. Given the strong correlation between AXTOT and water-unextractable arabinoxylans (WUAX) (r = 0.86, data not shown), the effect of AXTOT on P is probably attributable to WUAX, which is consistent with the results of Garófalo et al. (2011). This suggests that these minor components contribute to dough tenacity, as previously demonstrated in studies where bran or WUAX fractions were added to white flour (Bonnand-Ducasse et al., 2010; Gómez et al., 2003), possibly through a filler-like effect in the dough matrix, distinct from the impact of AX on water absorption.

Regarding lipids, total stearic acid content (C18.TOT) appears to have a negative impact on both W and DE. While its effect on W is minor compared to the other variables and can be overlooked, its effect on DE is more pronounced. Although the influence of C18.TOT is statistically significant, interpreting this result is challenging. However, the negative contribution of C181n9.TOT suggests a balance between several fatty acids to model DE. These results indicate that lipids play a more significant role in dough behaviour during resting and shaping—reflected by DE measurement—where reactions such as oxidation can occur. In contrast, oxidation reactions are probably limited during alveograph measurements, which may explain why Ie is not affected by lipids.

4.4. Modelling DE using alveograph variables

Our findings suggest that DE is most likely explained by alveograph variables, especially by Ie. To assess this hypothesis, the model selection procedure was run once again for DE, this time including alveograph variables as potential explanatory variables. The results of the BIC and VIF tests are given in Supplementary Fig. S5, and the selected models are reported in Table 3A. The resulting MOI, referred to as MA-DE_4 (Table 3A), shows that Ie has a strong negative effect on DE, with P having a lesser impact, in addition to lipid-related variables (C18.TOT, C181n9.TOT and C183n3.TOT).

Models of Ie, P and W (M-IE_3, M-P_2, M-W_3) were used as latent variables to assess the influence of the flour composition on DE and, more generally, on the dough's stretching capacity. The resulting MOI, referred to as Ma-DE_1 (Table 3B), shows that DE can be modelled by M-Ie_3 and GluS. As expected, GluI is not included in this model since its impact on the gluten network is captured by M-Ie_3.

The predicted vs. the actual values of DE for the three DE models—Ma-DE_1 ($R^2_{CV} = 0.65$), M-DE_5 ($R^2_{CV} = 0.68$), MA-DE_4 ($R^2_{CV} = 0.79$)—are shown in Fig. 3. The predictive performances of M-DE_5 and Ma-DE_1

Table 3

Models selected on the basis of Bayesian Information Criterion (BIC) and Variance Inflection Factor (VIF) tests for Dough Elongation at shaping (DE) with: A) composition and measured alveograph variables (incl. WAM); B) with composition and predicted alveograph variables (M-Ie_3, M-W_3 and M-P_2).

A)	Protein variables		Arabinoxylans variable	Lipids variables			Technological variables				Statistical metric values		
	GluI	Gli	AXTOT	C18.TOT	C181n9.TOT	C183n3.TOT	W	Ie	P	WAM	n[a]	R^2cv	BIC score
MA-DE_{Ie}								−0.86			1	0.74	−376.9
MA-DE_1			−0.12					−0.88			2	0.75	−387.0
MA-DE_2		0.21					−0.25	−0.80			3	0.76	−394.5
MA-DE_3	−0.27	0.18	−0.13					−0.77			4	0.78	−405.9
MA-DE_4				0.17	−0.15	0.21		−0.84	−0.19		5	0.79	−421.1
MA-DE_5		0.23		0.20	−0.15	0.18		−0.95		−0.26	6	0.80	−427.0

B)	Protein variables		Damaged Starch variable	Arabinoxylans variable	Lipids variable	Predicted variables		Statistical metric values		
	GluS	Gli	SD	IV.AX	C181n9.TOT	M-Ie_3	M-W_3	n[a]	R^2cv	BIC score
Ma-$DE_{M\text{-}Ie3}$						−0.81		1	0.64	−290.9
Ma-DE_1	0.14					−0.86		2	0.65	−290.9
Ma-DE_2	0.20	*0.24*	0.27	0.23			−1.04	5	0.69	−312.5
Ma-DE_3	0.20	0.26	0.27	0.22	*−0.07*		−1.02	6	0.69	−310.0

Variables were standardised for each linear regression model and their corresponding coefficients are indicated. Terms in the models considered not significant (p-value ≥0.001) are in italic. The models are ranked in ascending order of predictive performance, the ranking being indicated in the form of indices, except for the univariate model, which mentions the name of the variable. Grey-shaded model is the Model Of Interest (MOI). The BIC score indicated is the difference between the BIC from the model and the BIC from the control i.e the mean value of the response variable.

GluS: Soluble Glutenin content; GluI: Insoluble Glutenin content; Gli: Gliadin content; SD: Damaged starch measured by iodine absorption; AXTOT: Total arabinoxylan content; IV.AX: Intrinsic viscosity from water-extractable arabinoxylans; C18.TOT: Total stearic acid C18 content; C181n9.TOT: Total oleic acid C18:1n-9 content; C183n3.TOT: Total alpha-linolenic acid C18:3n-3 content; W: Baking Strength, Ie: Elasticity Index; P: Tenacity; WAM: Water Absorption simulated from protein content, Soluble Starch, Damaged Starch, and Specific Viscosity from water-extractable arabinoxylans, M-Ie_3: Ie simulated computed from Insoluble Glutenin content, Soluble Starch, Damaged Starch and arabinose on xylose ratio, M-W_3: W simulated from Insoluble Glutenin content, Total stearic acid C18 content and WAM.

[a] Number of variables included in the model. BIC: Bayesian Information Criterion. VIF: Variance Inflection Factor.

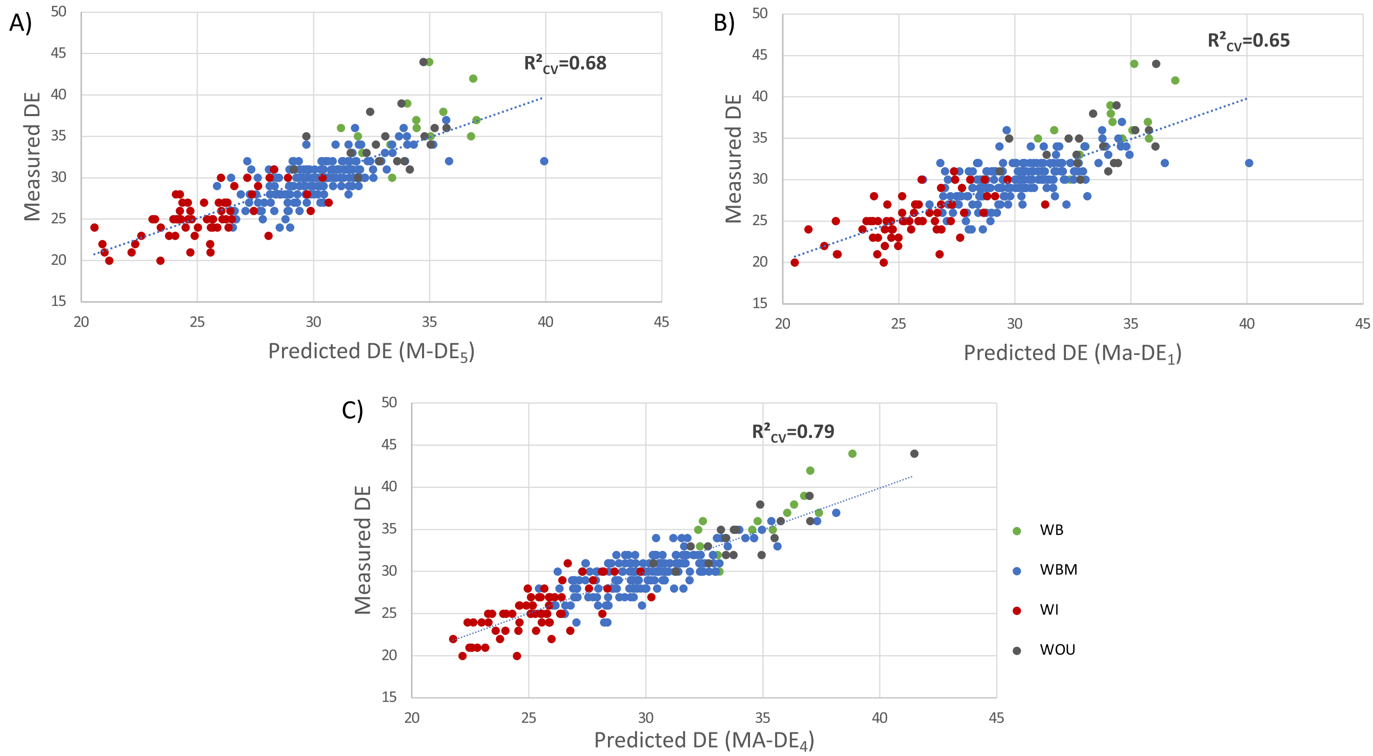

Fig. 3. Comparison of the prediction of dough elongation at shaping (DE) against measured values for the models (A) M-DE$_5$; (B) Ma-DE$_1$; and (C) MA-DE$_4$. Displayed predicted values are selected from the fraction of data used for model validation during K-fold cross validation. The corresponding coefficient of determination, denoted R^2_{CV}, is reported. The legend indicates the intended end-uses of the wheat samples.
M-DE$_5$ $= \beta_0+\beta_1*$**GluI**$+\beta_2*$**C18.TOT**$+\beta_3*$**GluS**$+\beta_4*$**IV.AX**$+\beta_5*$**C181n9.TOT**
Ma-DE$_1$ $= \beta_0+\beta_1*$**M-Ie$_3$**$+\beta_2*$**GluS**
MA-DE$_4$ $= \beta_0+\beta_1*$**Ie**$+\beta_2*$**C183n3.TOT**$+\beta_3*$**P**$+\beta_4*$**C18.TOT**$+\beta_5*$**C181n9.TOT**
WB: Wheat for Biscuit applications; WBM: Wheat for Bread-Making applications; WI: Improver Wheat; WOU: Wheat for Other Uses.

are similar, both reflecting the variability in DE that can be explained by composition variables, which are largely related to dough elasticity, measured by Ie. However, MA-DE$_4$ outperforms the other two models, particularly in predicting the high DE values observed in the wheat used for biscuit applications (WB). This finding shows that, while the composition measurements in the dataset account for most of the DE variability, incorporating alveograph measurements significantly enhances the prediction of dough behaviour during the manufacturing process. These results lead to another representation of interaction between all these components, technological variables and quality indicators (See Supplementary Fig. S6).

Predictive tools such as the alveograph are commonly used to assess dough behaviour, but the bread-making test, which reflects real manufacturing conditions, remains the ultimate benchmark despite being time-consuming. In this context, DE is particularly interesting. However, it is less accurately predicted than Ie or W, suggesting a weaker dependence on flour composition. This may be due to the fact that DE is measured at the dough's optimal hydration level, whereas alveograph measurements are performed under sub-optimal hydration. The increased hydration probably reduces the sensitivity of DE measurements to flour composition. Although bread volume (BV), is a key quality criterion in the bread-making test, we were unable to obtain a reliable regression model for BV using the present dataset.

Overall, L and P/L proved challenging to predict, which has been observed in previous studies (Branlard et al., 2013). This suggests that L might reflect a combination of intertwined mechanisms that are difficult to account for using composition data alone. L measures the maximum extension of the dough bubble before it bursts. While it is positively correlated with proteins, especially GluS, it is negatively correlated with P, which is highly dependent on WA. It could therefore be inferred that a lack of water results in a tougher dough (high values of P) that burst more quickly.

5. Conclusion

This study demonstrates that flour composition—including major components (proteins and starch) and minor ones such as arabinoxylans and lipids—plays a critical role in shaping dough behaviour. Among the technological variables examined, the elasticity index (Ie) emerged as the most informative predictor of dough elongation (DE), underlining its value for assessing dough quality.

Our findings further confirm that DE, a quantitative measure of dough extensibility during shaping, is a robust and well-predicted bread quality indicator within the French bread-making context. In contrast, bread volume (BV)—considered a key indicator of baking quality in many countries—proved more difficult to predict.

While Ie and DE are strongly influenced by GluI, DE is also affected by GluS and possibly by lipids. In contrast with P or W, both Ie and DE are unaffected by WA. The underhydrated state of the dough during alveograph measurements is evident, as shown by the dependency on water absorption of P and W. Ultimately, the best model for predicting *DE* primarily relies on technological variables, with *Ie* as the main contributor and *P* playing a lesser role, in addition to a minor contribution from lipid-related variables.

Minor components are often overlooked when analysing the natural variability of wheat characteristics in relation to bread-making performance. However, arabinoxylans have been shown to impact water absorption and, as demonstrated in this study, significantly affect dough behaviour through the effect of WEAX on water absorption and potentially through the direct mechanical impact of WUAX on the gluten network. Similarly, lipids have been identified as having a significant impact on dough behaviour, underscoring the importance of considering these components when assessing wheat quality.

For the cereal sector, these findings provide new leads for improving flour functionality prediction, reducing reliance on time-intensive baking tests and supporting wheat classification and selection strategies aligned with modern processing constraints and consumer expectations.

CRediT authorship contribution statement

Laura Rezette: Writing – original draft, Visualization, Investigation, Formal analysis, Data curation. **Luc Saulnier:** Writing – review & editing, Visualization, Supervision, Project administration, Methodology, Funding acquisition. **Marie-Hélène Morel:** Writing – review & editing, Methodology, Investigation. **Benoît Méléard:** Writing – review & editing, Methodology, Investigation. **Sophie Le Gall:** Writing – review & editing, Supervision, Methodology. **Kamal Kansou:** Writing – review & editing, Visualization, Supervision, Methodology, Formal analysis.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jcs.2025.104233.

Data availability

The dataset used in this work is accessible through the link https://doi.org/10.1016/j.dib.2025.111375.

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Glossary

AX: Arabinoxylans
A/X.TOT: Arabinose-to-Xylose ratio from Total Arabinoxylans
AXTOT: Total Arabinoxylans
A/X.WE: Arabinose-to-Xylose ratio from Water-Extractable Arabinoxylans
BIC: Bayesian Information Criterion
C16.TOT: Total palmitic acid C16 content
C18.TOT: Total stearic acid C18 content
C181n7.TOT: Total vaccenic acid C18:1n-7 content
C181n9.TOT: Total oleic acid C18:1n-9 content
C182n6.TOT: Total linoleic acid C18:2n-6 content
C183n3.TOT: Total alpha-linolenic acid C183n-3 content
CV%: Coefficient of Correlation
DE: Dough Elongation at shaping
IE: Elasticity Index
Gli: Gliadin content
GluS: Soluble Glutenin content
GluI: Insoluble Glutenin content
IV.AX: Intrinsic Viscosity from Water-Extractable Arabinoxylans
L.: Extensibility
MOI: Model of Interest
P: Tenacity
Prot: Protein content
SS: Soluble Starch
SD: Damaged Starch measured with SD-Matic (iodine absorption)
SV.AX: Specific Viscosity from Water-Extractable Arabinoxylans
VIF: Variance Inflection Factor
W: Baking Strength
WA: Water Absorption
WAM: Predicted Water Absorption with Prot, SS, SD and SV.AX
WEAX: Water-Extractable Arabinoxylans
WB: Wheat for Biscuit applications
WBM: Wheat for Bread-Making applications
WI: Wheat used as Improvers
WOU: Wheat for Other Usages
WUAX: Water-Unextractable Arabinoxylans
WUAX: Water-Unextractable Arabinoxylans