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One Model to rule them all: Developing Universal Aquaculture feed composition models.

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ABSTRACT

Ensuring the aquaculture feeds (aquafeeds) meet the expected nutritional and physical specifications is paramount in research and commercial aquaculture. This approach reduces the risk of experimental failure and costly rework as well as the disposal of unsuitable commercial diets. This study aimed to produce a single NIR model capable of predicting the proximate composition and starch damage of aquafeeds. We had access to a historical library of samples (ingredients and diets), as well as manufacturing diets (extrusion and steaming). The diets were ground before scanning by NIRS, then models were developed to estimate dry matter, ash, lipid, protein, and energy as well as starch damage. Proximate prediction models were successfully produced for diets and ingredients with R2 values between 0.88 and 0.97, while starch damage models were produced with R2 values between 0.91 and 0.97. The developed NIR models allow to rapidly monitor the nutritional composition, as well as one of the main physical properties of the diets before undertaking experimental work. These models could be used by any aquaculture laboratory and aquafeed company wanting to have a rapid quality control check of their diets.

INTRODUCTION

Production of aquafeeds is an expensive exercise both in the cost of resources and in man-hours. Currently, checking whether aquafeeds meet or not the expected formulations by classical chemistry methodology is time-consuming. This is a common concern in research and commercial feed manufacturing facilities. For example, a failure of an experiment due to inaccurate diet composition will require repeating, doubling its expected cost. Whilst, for commercial feed companies producing tons of feed per hour nonstop, the benefits of adjusting formulation inaccuracies in real-time as opposed to days later are enormous. Optimisation of workflow and improvements in quality control in these facilities can help to reduce these costs.

This study aimed to produce a single NIR model capable of predicting the proximate composition and starch damage of aquafeeds to reduce lead-time required between diet manufacturing and quality control approval checks.

METHODS AND MATERIALS

To prepare the diet calibration, a set of 60 diet samples were selected from a historical library of samples produced for previous work (ingredients and diets) to cover a range of aquatic species. A total of 83 ingredients used in the preparation of those diets were used for the NIR ingredient calibration. For the starch cook prediction model, five basic aquafeed formulations with increasing starch content and different botanical sources (wheat, tapioca, rice, and potato) were prepared. For each formulation, thirty kilograms of each mash was made before being subsampled for different diet manufacturing processes (extrusion and steaming) relevant for fish and prawns. The mash feed rate, moisture addition, and screw speed were manipulated to give a range of different samples, with varying specific mechanical energy (SME) inputs and different levels of gelatinisation/cook. The samples were ground to pass through a 750 micron screen before being subjected to NIR analysis.

Spectroscopy and analysis:

The samples were scanned using a Pertin DA7200 Diode Array NIR Spectrometer. The samples were then scanned in reflectance mode over wavelengths from 950 nm to 1650 nm at 1 nm intervals and their spectra recorded. A total of 6 scans were completed for each sample, 3 prior to, and 3 after repacking. All scans were done at room temperature, ~24°C, with the sample, rotated while scanning to increase sample exposure to the NIR instrument. Background corrections were taken before each scan and the average of all recorded spectra for each sample was used in the preparation of the models.

Partial least squares (PLS) regression was used in the construction of the near infrared spectra models using the Unscrambler X software (Camo, version 10.3). The raw scans were subjected to several pre-treatment options including area normalisation (AN), smoothing (S), first derivative (1D), and a combination of the former. Random segmented cross-validation was used during model construction using 20 segments at 7 samples per segment.

The statistics calculated for assessing the robustness of the calibration models included the number of principal components (PCs), the correlation coefficient between predicted and measured composition (R2), and the standard error of cross-validation (RMSECV). RMSECV is the standard deviation of differences of the residuals between the NIRS and chemically determined concentrations and has been reported to be the best estimate for the prediction capability of calibrations (refs). The best models were selected based on the lowest RMSECV and the highest R2 of the cross-validations. The residual predictive deviation (RPD) was calculated as the standard deviation of the measured composition (SD) divided by the RMSECV to evaluate the performance of the calibrations.

RESULTS

Prediction models were successfully produced for diets and ingredients which showed the coefficient of determination of the measured and predicted values where R2 values were

greater than 0.88 and are suitable to be used for quality control analyses (Table 1). It should be noted that due to the chemical properties of the samples, it was necessary to only produce a nitrogen ingredient calibration vs a protein equivalent calibration for the diets.

A comparison of model predicted values to analytically measured values indicated that NIRS was able to provide fast and accurate checks of the chemical composition of diets, regardless of the method of manufacture or species. The NIR models were able to predict proximate composition within 1.5%, which is consistent with the accuracy achieved in the laboratory.

Starch damage models for both diet manufacture methods and a combined model were produced. The combined model used both extruded and steamed samples to produce a generic starch damage model. The model successfully predicted the degree of starch damage, with a R2 value of 0.915 and 5.76% SECV value for the cross-validation set. This high SECV value along with the RPD and RER values of 1.2 and 7.2, respectively, indicates the model is suitable for screening samples only. Models produced for the individual production methods show improvements in SECV, RPD and RER values that are somewhat suitable for process quality control. Thus the improvement of the models suggests that each type of diet pelleting process requires a dedicated model to provide more robust results.

CONCLUSIONS

We were able to produce models that allowed us to use NIR instead of analytical chemical methods for quality control checks on aquafeed proximate composition and starch damage, saving both time and money by reducing the lead-time between experimental diet manufacturing and trial commencement, as well as using them for near-realtime adjustment of feed composition for commercial operations.

TABLE 1. NIR Model Statistics.

Component	Transformations	PCs	R^2	SECV	RPD	RER	Validation	Validation Error
Ingredient Prediction Models								
Dry Matter	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 49 Samples	9	0.909	0.74	9.1	55.8	0.870	1.15
Ash	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 70 Samples	5	0.909	1.40	4.8	29.6	0.905	1.62
Lipid	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 83 Samples	5	0.967	1.97	3.4	21.0	0.888	2.64
Lipid	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 82 Samples	5	0.883	1.93	3.5	21.5	0.863	2.32
Nitrogen	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 83 Samples	6	0.913	1.32	5.1	31.3	0.902	1.55
Energy	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 71 Samples	4	0.893	2.05	3.3	20.2	0.879	0.86
Diet Prediction Models								
Lipid	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 67 Samples	5	0.959	0.74	9.2	56.3	0.954	0.85
Ash	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 101 Samples	13	0.954	0.75	9.0	55.4	0.903	1.09
Energy	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 81 Samples	5	0.919	0.43	15.6	95.9	0.897	0.50
Protein	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 69 Samples	9	0.973	1.46	4.6	28.3	0.958	1.90
Dry Matter	Smoothing:SG, 2nd order, 9 points; Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 950-1650; 68 Samples	8	0.894	0.62	10.9	66.7	0.775	0.89
Diet Prediction Models								
% Starch Damage	Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 954-1646; 149 Samples	10	0.915	5.76	1.2	7.2	0.870	7.77
% Starch Damage Steamed	Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 954-1646; 19 Samples	5	0.976	3.68	1.8	11.2	0.934	5.89
% Starch Damage Extruded	Area Normilisation; 1st Driv, SG 2nd order, 9 Smoothing; 954-1646; 1111 Samples	9	0.919	3.60	1.9	11.5	0.919	4.77