Simulation of yield and quality of malting barley

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Abstract

A computer simulation model was developed to determine the likely response of grain yield and quality of malting barley crops to differing availability of water or nitrogen (N) and differing soil and climatic conditions. The model was validated for New Zealand conditions by comparing the results of model simulations with data from malting barley crops grown in the Manawatu. Simulations were then performed to determine the best water and N management strategies for producing quality grain for malting (low N concentration and large grain size) as well as minimising the production risks and variability across seasons. Predictions were obtained for plant development, biomass production, and crop quality variables. Without irrigation there was a high risk of producing high grain N concentration, and therefore poor malting quality, irrespective of N management. With irrigation, the probability of producing grain with less than 2% N was greatly increased. Good quality grain could be produced even on high fertility sites or with high N inputs provided there was enough water to sustain growth processes at a near-optimal level.

Additional key words: *irrigation, nitrogen, modelling, response surfaces*

Introduction

Consistent high quality grain (< 2% N) for malt is difficult to achieve in high-fertility sites due to excessive N uptake early in development or late N uptake and subsequent mobilisation of N to developing grain, (de Ruiter et al., 1988). Therefore, a compromise must be reached to optimise quality and yet not sacrifice too much in grain yield by limiting the level of N in the crop. Progress has been made in simulation modelling of quality components such as N concentrations in grain and grain size in wheat (Sinclair and Amir 1992; van Keulen and Seligman, 1987) but few attempts have been made for barley. In the case of malting barley, these quality components are of prime interest to both farmers and processors, (Drewitt and Smart 1981, Smart 1983).

In shallow soils, the occurrence of water stress may contribute to an increased likelihood of shrivelled grain with high N concentrations (Drewitt and Smart, 1981; Stark and Brown, 1987). Also, under conditions of high nitrogen fertility and adequate soil water, reductions in grain quality may occur as a result of shrivelling, (Martin and Daly, 1993). Under these conditions grain nitrogen concentrations are also responsive to N application, (Martin and Daly, 1993). However, in a dryland situation, soil and climatic conditions which are conducive to reliable production of high quality grain are difficult to predict, (de Ruiter and Brooking, 1994a). In practice, N nutrition is a problem where water availability is variable because of soils with low water holding capacity or high vegetative growth causing high transpiration losses and an eventual loss in yield due to late stress, (Drewitt, 1883, Lawlor *et al.*, 1981). Near-ideal growth conditions are rarely if ever achieved and the consequence is that water shortage or nutrient deficiency may lead to serious yield or quality reductions. The basic processes underlying the relation between water availability and crop production, as well as the responses of crops to nutrient (more particularly nitrogen) availability are sufficiently well understood for functional relationships to be established and quantitative descriptions made. Consequently, there has been considerable development of models for major crops such as wheat and maize (Rickman and Klepper, 1991). For wheat, in particular, thorough studies on individual crop responses such as tiller number and nutrient level, grain yield and temperature has led to a good understanding at the process level, (Porter, 1984; Porter, 1985; Sadras and Connor, 1991).

Availability of water and N are central to crop production systems. In field situations, the interactions between the water and nutrient availability are complex and the integration of the processes into a dynamic model can aid in the analysis of growth, water use and N nutrition and their interactions under different and variable conditions. The development of explanatory simulation models for cereals has provided opportunities for analysis of production potentials of cereals (Stapper and Harris, 1989). Models of this nature provide a conceptual system with feedbacks that can explain interactions between environmental and management factors that occur during crop growth. Simulation modelling is also a promising means for testing the current concepts about the physiology and growth processes of cereal crops in response to varying conditions of water and nitrogen availability (Groot and Spiertz, 1991; van Keulen, 1991).

A number of published crop models have been used to predict variations in crop yield (Ritchie, 1991; Porter *et al.*, 1993). These models use an empirical approach for predicting biomass accumulation in primarily non-limiting growth situations. While many of these models predict biomass well, they are inadequate for processes that influence the allocation of reserves to the various plant organs. Grain quality variables such as grain size or grain nitrogen (N) concentration are more difficult to predict as they rely on the accurate partitioning of N and carbon, both through uptake/assimilation and redistribution.

The objectives of this study were to (a) develop a model for malting barley capable of predicting variation in grain quality and yield, and (b) simulate the effects of variation in water availability and N uptake on yield and evaluate possible management options which may lead to a more stable productivity and quality of grain for malting.

The Model

The spring wheat model (SWHEAT) of van Keulen and Seligman (1987) was used as a framework for the development of a barley model (BARLEY). The wheat model was developed as part of a project to study production potential in a semi-arid Mediterranean environment so it focused on situations where either the supply of water or the availability of N was a limiting factor for production. The BARLEY model was designed to account for the effects of varying moisture and N availability on the growth and organ formation of barley. Neutral soils were assumed with N being the only nutrient deficiency. Limiting factors other than water or nutrient, such as weed competition, pests and diseases were not accounted for.

BARLEY is essentially a mechanistic simulation of the dynamics of moisture and N in the soil, their availability to the crop and accumulation of dry matter and nitrogen in various organs. Crop growth dynamics are based on parameters for photosynthetic performance, organ formation, and distribution of assimilate and N among the various plant organs in relation to phenological development. Most functions in the model are formulated to account for moisture and N stress at any point in the growth cycle.

Daily meteorological inputs needed to run the model are maximum and minimum temperature, solar radiation, and rainfall. Additional plant inputs are required to define the distribution of assimilates among various plant organs in relation to development stage, the leaf weight/area ratio, root development, assimilate requirements for the formation of various plant organs, maximum levels for N concentration in the different plant organs and functions defining rate of phenological development. Soil physical data are required because they determine the amount of plant available water. These include the soil moisture contents at field capacity and wilting point. To complete the N balance, inputs are required for the amount of stable N and carbon in the soil organic matter and crop residues.

An option is available for the selection of autumn or spring sowing. For autumn sowing, the degree of vernalisation is expressed by a delay or advance in development due to a reduced rate of thermal time accumulation and the satisfaction of a photoperiod requirement for vernalisation. The model of Reinink *et al.* (1986) was used to define the vernalisation response.

The model runs under a FORTRAN-77 Simulation Environment allowing flexibility for input of weather data, input of soil and plant variables, and convenient graphical or tabular output. Finer details of the FORTRAN Simulation Environment (FSE) are given in Rappoldt & van Kraalingen, (1990); van Kraalingen, (1991) and van Kraalingen *et al.* (1991).

Model performance was assessed in a series of calibration simulations with adjustments for processes governing vernalisation and photoperiod sensitivity, development rates for pre- and post-anthesis growth phases, potential growth rate of individual grains, assimilate supply allocation to the various organ pools, and relationships between leaf N content and photosynthesis. Calibration data were obtained from an early sowing of an experiment conducted at Aorangi in 1987/88 (de Ruiter and Brooking, 1994b). This experiment was used to provide plant inputs, historical meteorological data and data for N management. A single application of 60 kg N/ha was applied at sowing (18 September). Additional soil inputs were required to characterise the soil environment and were typical of a Manawatu sandy loam. These included the initial weight of stable organic material (HUMI) in the soil profile (90 000 kg/ha), initial weight of N in the stable soil organic material (NHUMI) (9 000 kg/ha), level of N in soil microbial biomass (IBIOMN) (20 kg/ha), and distribution factors for stable and fresh organic material in the soil profile (all in the top 80 cm).

A more detailed description of development and calibration of the model will be published in a separate paper.

Model Validation

Data from a sowing date trial conducted in the 1988/89 season at Aorangi were used for model validation. Crops were sown on four dates approximately three weeks apart beginning 27 September and ending 5 December. The experiment was arranged in a randomised complete block design. Each sowing date main plot was randomly divided into nil or 50 kg N/ha treatments. N was applied in the form of urea at tillering.

Validation results showing the observed and simulated values are given in Table 1. Predicted biomass yields were lower than the observed values except for the late sowing. There was no clear reason for the under-prediction of biomass yield, although it was possible that the reduction of leaf growth in response to water deficit was too sensitive. Another possibility was that the amount of soil moisture available for growth was limiting because of under-estimation of the calculated water reserves. Root growth proceeds at a predefined rate in the model but may not keep pace with the rapid loss of water through soil evaporation.

Predictions of grain yield were lower than the experimental values, except in the late sowing. In the second and third sowing, under-prediction of grain yield could have resulted from inadequate description of processes controlling total tiller production, tiller numbers per plant, grains numbers per unit area, or weight per grain. All these variables showed some deviation between observed and expected data. The onset of water stress conditions during grain filling, particularly in sowings two and three, may explain some of these deviations.

Table 1. Comparison of simulation model predictions (pre) with experimental observations (obs) for dry matter and yield component variables at Aorangi.

		Sowing Date							
		1 (27/9)		2 (17/10)		3 (8/11)		4 (5/12)	
		-N	+N	-N	+N	-N	+N	-N	+N
Total above ground dry weight (t/ha)	obs	11.20	12.08	10.37	11.06	9.50	9.56	6.75	6.45
	pre	11.16	11.41	9.58	9.59	7.81	8.04	9.12	8.73
Grain Yield (t/ha)	obs	5.10	5.29	4.53	4.75	3.76	3.57	2.21	1.93
	pre	5.08	5.03	3.39	3.40	3.52	3.60	4.92	4.72
Harvest Index	obs	0.46	0.46	0.44	0.43	0.39	0.37	0.32	0.30
	pre	0.46	0.44	0.35	0.35	0.45	0.45	0.54	0.54
Tiller number per m^2	obs	809	834	758	800	783	796	894	898
	pre	955	1012	717	727	739	734	589	552
Tillers per plant	obs	2.8	2.7	4.1	4.3	2.5	2.6	3.2	3.1
	pre	3.3	3.2	3.9	3.9	2.3	2.4	2.0	2.0
Grain number per m^2	obs	15740	17060	14594	15008	15645	15922	11396	10204
	pre	19374	20855	10106	10314	14527	13969	11436	10900
Thousand grain weight (mg)	obs	32.4	31.0	31.1	31.7	24.0	22.4	19.5	19.0
	pre	26.2	24.1	33.6	33.0	24.2	25.8	43.1	43.3
Grains per ear	obs	19.5	20.5	19.3	18.8	20.0	20.0	12.8	11.4
	pre	20.4	20.7	14.3	14.4	19.9	19.2	19.5	19.9

There was considerable deviation between observed and predicted grain size in sowing 4, (Table 1). The validation crop developed severe leaf rust during early grain-filling which was not accounted for by the model. Predictions therefore indicated potential productivity in the absence of the disease. The general decline in productivity in both the observed and predicted data with the later sowings was a result of the declining availability of soil moisture.

The effects of N availability were unclear in these simulations. Significant responses to added fertiliser N occurred in the experimental plots, but these were not predicted in the simulations. Simulated rates of N mineralisation from organic matter were possibly too high. Plant N uptake was therefore occurring at 'near maximum' rate regardless of fertiliser application rate. Total N in the above ground biomass (TNABM) was overpredicted although N allocation to grain was similar in the simulation and validation crops, (Table 2). This resulted in under-prediction of N harvest indices for the first three sowing dates. In spite of low N harvest indices, the concentration of N in the grain was higher in the simulation than in the observed treatments, a reflection of the excessive N uptake in the model. Precise description of the levels of inorganic N at the onset of simulation and the rates of mineralisation during growth were also important to determine the likely responses under varying management.

The total N accumulation in the grain (WGR) was predicted reasonable well, but N harvest indices were abnormally low. There was the possibility that the partitioning processes for N, and possibly dry matter as well, may require further calibration. N concentrations in the grain were higher than expected, indicating more than adequate rates of N mobilisation from stem reserves. The distribution of N also indicated that improved calibrations were necessary to predict the N balance in the plant at the end of the season, particularly in situations where high amounts of N are accumulated in the herbage.

Model Prediction

Given that the model performed satisfactorily in the New Zealand environment, it was used to perform a series of simulations that would give some indication of the variability in yield and quality components.

The model was used for two sets of analyses. In the first it was used to simulate crop performance for three locations (Manawatu, Canterbury and Southland) with comparable soil fertility, and using up to 19 years of historical weather records to evaluate the variation induced by seasonal fluctuation alone. In the second set, the effects of a range of soil water and N availabilities in a Manawatu environment were examined. Response surfaces for growth and quality characteristics were developed by repeat simulations with either 5 July 1994 supplementary irrigation or simulated deficit, or water deficit with varying N fertility.

Long-term simulations

Climatic variability from year-to-year is one of the prime causes of variation in crop performance. Historical weather records were used to simulate the variation among seasons for three sites in New Zealand, with model starting values as for the Aorangi (Manawatu) validation. The data in Figures 1, 2 and 3

Table 2. Comparison of simulation model predictions (pre) with experimental observations (obs) for N response variables at Aorangi.

		Sowing date							
		1 (27/9)		2 (17/10)		3 (8/11)		4 (5/12)	
		-N	+N	-N	+N	-N	+N	-N	+N
Total N in the above ground biomass ($g.m^2$)	obs	12.1	14.6	13.9	16.9	11.8	14.7	12.1	12.3
	pre	23.5	24.7	21.9	22.7	17.7	18.5	16.1	15.6
Amount of N in the grain (g/m^2)	obs	9.2	10.9	9.2	11.1	7.1	8.6	5.3	4.5
	pre	11.7	11.7	8.7	9.0	8.8	8.7	7.7	7.9
Nitrogen Harvest Index	obs	0.71	0.69	0.62	0.60	0.59	0.53	0.40	0.35
	pre	0.50	0.47	0.40	0.40	0.50	0.47	0.48	0.51
Fraction of N in the grain (%)	obs	1.67	1.89	1.89	2.14	1.84	2.17	2.20	2.28
	pre	2.31	2.31	2.57	2.64	2.49	2.40	1.56	1.68

are examples of the ranges of predicted grain yield, grain size and grain N concentration, respectively, with the assumption that fertility and water holding capacities (150 mm) of soils in the three locations were similar. The modelled responses therefore indicated the likely variation imposed by the climatic differences alone. The curves also indicate the risk involved in achieving a particular grain yield level, average grain size or N content, respectively.

Simulated potential grain yields were similar in all regions, but average yields were lower in Canterbury and Manawatu than in Southland. There was a 35% chance of exceeding a 6.0 t/ha yield in Canterbury compared with a 50% chance in Manawatu and a 90% chance in Southland. Probabilities of achieving an average grain size of 30 mg/grain were better the further south the crops were grown, although the predicted variation in size was greatest in Canterbury where the climate is more variable. Therefore, the risk of producing low yield and low grain quality was greater in this region. Canterbury and Manawatu also showed similar trends and probabilities for predicted grain N concentration. In both locations, N concentrations were expected to exceed 2% in 35% of years, whereas good quality grain (< 2% N) could be expected in all seasons in Southland. The above simulations were performed assuming no irrigation. Clearly, better quality could be achieved if there was more water available to support growth. The timing of available water was also considered to be important in the development of yield and quality.

Scenarios for water and N management

Simulations were performed to determine the responses of malting quality parameters (grain N concentrations and grain size) to water and N interactions. A range of treatments were formulated to observe the effects of varying water availability (approximating -30% to +50% deviation from the long-term mean soil water deficit (Fig. 4a). The range of water deficits was achieved by applying either a simulated irrigation or simulated drydown at 5-day intervals, beginning at day 50. The indicated level of irrigation or drydown (Fig. 4b) was distributed in amounts relative to the difference in soil water in the preceding 5-day period. This resulted in realistic simulated soil water extraction patterns (Fig. 4b) for the

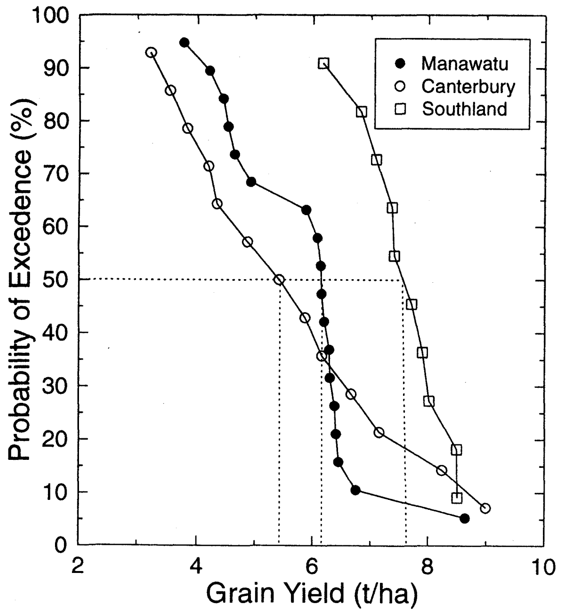

Figure 1. Predicted distribution of barley grain yield (t/ha) for three locations in New Zealand. Dotted lines indicate the 50% probability levels for achieving the designated yield.

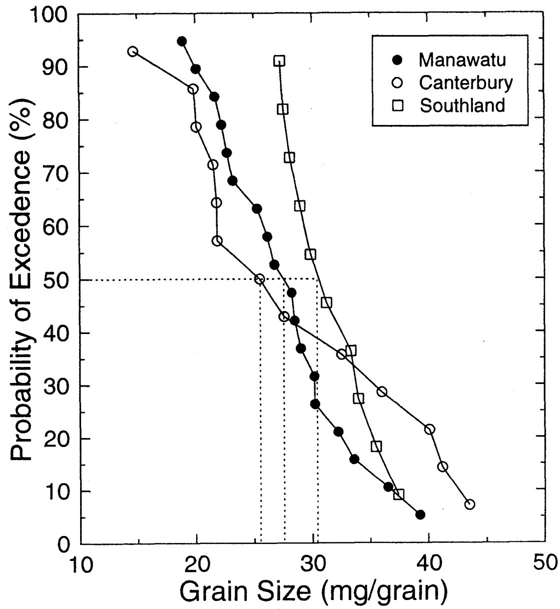

Figure 2. Predicted distribution of mean grain size (mg/grain) for three locations in New Zealand. Dotted lines indicate the 50% probability levels for achieving the designated mean grain size.

range of -200mm and +200 mm water withheld or applied. This range was similar to the proposed scenarios covering the -30% to +50% soil deficit range. Additional seasonal irrigations of 300 and 400mm were used to simulate near optimum situations of water availability. Calculations of soil water availability were based on a total profile capacity of 400mm, with a plant available capacity of 234 mm. The simulated soil water conditions were superimposed on four N fertility levels which were set up to simulate a range of 10 to 30 g/m^2 total N uptake, with an additional N application of 50 kg/ha at sowing for all treatments. Differences in available soil nitrogen were achieved by adjusting input variables for organic carbon (range 50,000 - 110,000 kg/ha); N in the organic soil fraction (5,000 - 11,000 kg/ha); inorganic N at sowing (30 - 60 kg/ha); and relative rates of decomposition of organic matter. The soil N levels (1 to 4), (Figs. 5 and 6) covered the range of fertilities for soils that were extensively cropped and the principle source for N from fertiliser to those newly out of pasture. Repeat simulations at fertility levels defined as input variables resulted in crop N uptakes of 9.8 to 30.4 g N/m^2, which were close to the proposed scenario range.

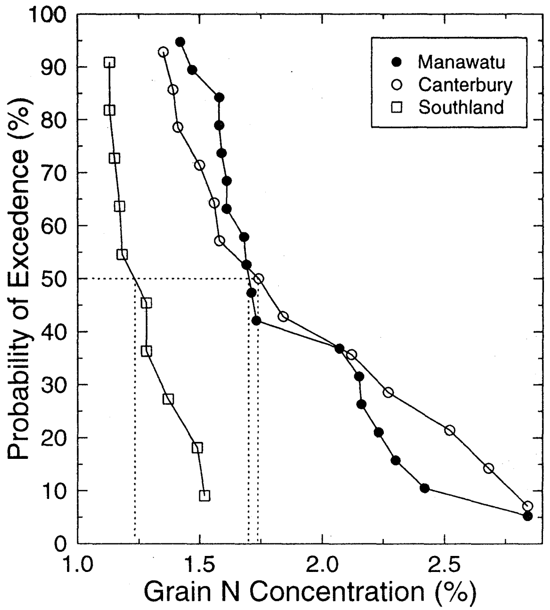

Figure 3. **Predicted distribution of barley grain N concentration (%) for three locations in New Zealand. Dotted lines indicate the 50% probability levels for achieving the grain N concentration.**

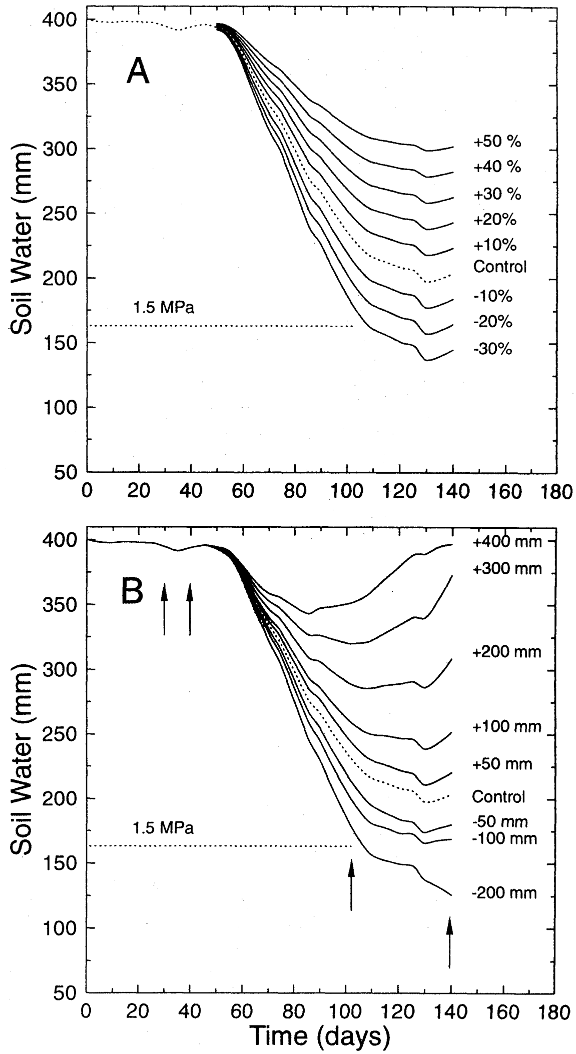

Figure 4. **Scenarios of soil water deficits spanning the range of -30% to +50% as calculated from 19-year mean soil conditions in the Manawatu (A). The soil water patterns in B, resulted from crop simulations with the indicated levels of total water applied or withheld during the season. Arrows indicate sowing, emergence, anthesis and maturity.**

The simulations were for a Manawatu environment and described the range of likely responses if rainfall was greater or less than the 19-year mean. It is inappropriate to discuss the complete set of crop variable responses to water and nitrogen. Therefore, a reduced data set is presented here, comprising predictions for grain N concentration and grain size alone. Scenarios of crop water use for simulated conditions of soil water availability deviating by -30% to +50% of the long term mean conditions corresponded with seasonal crop transpiration levels covering the range of 225 mm to 525 mm.

Generated response surfaces for grain N concentration, (Fig. 5) showed that in an average season without irrigation (simulated irrigation = 0), the risk of producing high grain N was high, particularly at the intermediate and higher soil N fertility levels. In seasons with marginally drier conditions the risks were even greater. However, with added water, the risk was substantially reduced, and grain N concentrations greater than the critical 2% were less likely to occur irrespective of N management (fertility level). The simulation results therefore indicated that good quality grain will be produced even in highly fertile conditions, provided that there is enough water to sustain growth at a near-optimal level.

Water availability had a near-linear effect on the simulated mean grain size, except for a small reduction of size at low soil fertility (Fig. 6). At low soil N availability there are probable limitations on leaf area expansion and therefore a limitation on the availability of carbohydrate to fill grains to their potential. This effect was not observed when 50 kg/ha N was applied at tillering or stem elongation in addition to that at sowing (data not shown). In comparison to water effects, site fertility had only a small influence on grain size. It was unlikely that the levels of soil water deficit caused a reduction in numbers of florets formed and subsequent grain number. Potential grain numbers are set by the mid tillering stage (around day 80, or 50 days after sowing), a time when the simulated soil deficits were less than 125mm. It remains to be determined whether the simulated grain size was responsive in situations where grain numbers are modified by the level of available N (or water) early in development when their effects may be more pronounced. Grain number may be responsive to sowing rate, but this possibility was not evaluated in these initial simulations.

The desired grain quality (grain N concentration or grain size) can be determined by matching the level of water availability and fertility with the appropriate response surface (Fig. 4), for soil moisture content. In

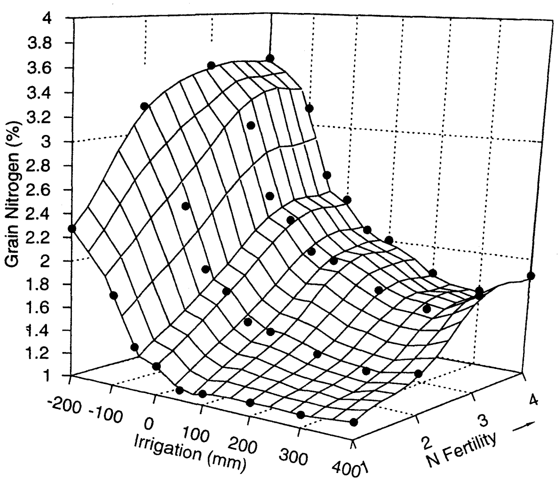

Figure 5. Simulated water x N fertility interaction for grain N concentration at Aorangi, Manawatu. Simulated soil water levels were as shown in Figure 4B.

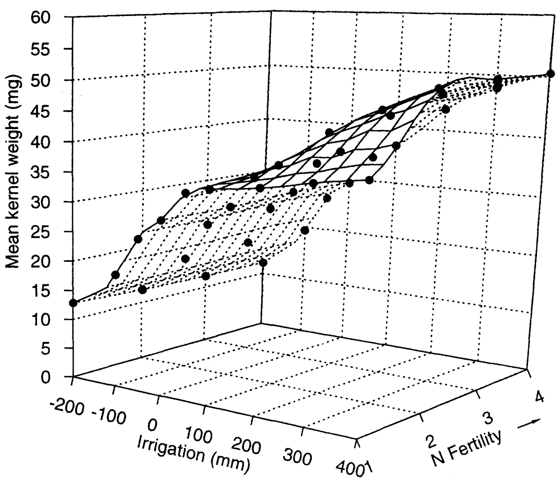

Figure 6. Simulated water x N fertility interaction for grain size at Aorangi, Manawatu. Simulated soil water levels were as shown in Figure 4B.

addition, it is possible to determine the likely irrigation requirement, for a given fertility level, to achieve a desired combination of grain yield and quality. At the low N fertility, simulated grain yields ranged from 2.8 to 8.3 t/ha for the given range in soil water availability. Similarly, at high N fertility the range was 2.7 to 11.2 t/ha.

Discussion and Conclusions

Crop model development must draw on the wealth of information already available (Muchow and Bellamy, 1991) and must also be sufficiently detailed to allow the model to explain the myriad of environmental and crop interactions. The published SWHEAT model of van Keulen and Seligman (1987) satisfied both these criteria and therefore formed a good base for the development of a model suitable for predicting the yield and quality responses of malting barley. The BARLEY model provided a means for analysing the effects of soil moisture availability and N fertility on the growth and grain yield of spring-sown malting barley in New Zealand conditions. SWHEAT was developed for semi-arid environments where interseasonal variation and distribution of rainfall cause dramatic fluctuations in dry matter and grain yields. Conditions in the Manawatu or Canterbury regions were not as extreme, but the underlying principles of crop water use and N use were appropriate.

Acceptable progress was made with BARLEY model development as realistic predictions were achieved for grain quality variables. The model is 'physiologically-based' and contains routines to handle turnover and accumulation of carbohydrate and N components in both the structural and reserve fractions. Therefore, the model is useful as a research tool to improve understanding of processes contributing to yield and quality formation. It also has considerable potential as a predictive tool to aid in crop risk evaluation, assessment of potential productivity in water and N-limiting environments, yield and quality variability assessment and in climate studies.

A validated model can be coupled with historical weather and soil data to provide a long-term series of dry matter, grain yield and quality simulations for a given site (region) as a function of different N and water regimes. Historical climatic records are also useful for determining the probability of crop failure or crop performance due to weather variability alone. The examples of site effects given in this paper demonstrate the effects of variability in climate and the subsequent effects on crop performance. This was extended to simulations of crop performance over a wide range of soil water and soil nitrogen availabilities. Simulations of this nature yields important information relating to the sensitivity of crop parameters to environmental perturbations. These simulations are also potentially useful for constructing databases for computer-based crop decision support aids for use in cropping situations where soil water and nitrogen are critical to attainment of a desired yield and quality range.

Ongoing model calibration and validation is required for improved prediction of barley performance under New Zealand conditions. The model, as yet, has not been fine-tuned for specific cultivar responses, although it can be easily adjusted for differences in development rate. The model needs to be calibrated over a wide range of conditions before it can be used with confidence to evaluate and assess the potential variation in yield and quality due to environment or resource limitations. Progress to the model prediction phase depended on the adequate description of crop performance as determined by the preceding calibration and validation phases. There were still deficiencies in the model performance after these phases, but the general responses were within the bounds of variation that could be expected in a field environment. The data used in calibration and validation were not from experiments specifically designed for that purpose, and therefore deviations between the simulated and experimental results were expected. Experiments are planned that will provide the appropriate data for a more precise calibration.

The ability to predict grain quality components correctly depends on adequate descriptions of specific details of carbon and N economy, and the fluxes and turnover of carbon and N through to the end of the growth cycle. The descriptions of the processes of carbon and N assimilation in the van Keulen and Seligman (1987) spring wheat model provide the detail necessary to achieve these goals, as they rely on the light-driven photosynthetic processes in a multi-layer crop canopy, and multi-layer soil processes affecting the uptake of N and crop N nutrition.

In summary, the model has potential for evaluating processes contributing to yield and quality formation, and as a predictive tool to aid in crop risk evaluation and assessment of crop performance in water and N-limiting environments.

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