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Optimization of fertilizer recommendations using response surface methodology and crop simulation models

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Abstract

The challenge of prescribing site-specific fertilizer rates for wheat has persisted for decades despite thousands of response trials worldwide. This research combined Response Surface Methodology (RSM) with the DSSAT-CERES wheat simulation model to optimize nitrogen (N), phosphorus (P), and potassium (K) recommendations for winter wheat at the University of Hohenheim experimental station, Stuttgart, Germany, during 2021-2023. A Box-Behnken design with three factors at three levels (N: 80, 140, 200 kg/ha; P₂O₅: 30, 60, 90 kg/ha; K₂O: 20, 50, 80 kg/ha) was implemented in field trials. RSM explained 91.3% of yield variance ($R^2 = 0.913$), with N as the dominant factor accounting for 62.4% of the response. The RSM-optimized combination (N: 168, P₂O₅: 72, K₂O: 54 kg/ha) predicted a maximum yield of 6.47 t/ha, which was validated by DSSAT at 6.31 t/ha (2.5% deviation). The integrated approach achieved a net return of EUR 847/ha, outperforming both blanket recommendations (EUR 714/ha) and farmer practice (EUR 623/ha). This framework offers a reproducible method for deriving location-specific fertilizer prescriptions that balance agronomic yield and economic return.

Keywords: Response surface methodology, crop simulation, DSSAT, fertilizer optimization, wheat, Box-Behnken design, nitrogen, phosphorus, potassium, precision nutrition

Introduction

Here's the challenge facing agronomists: blanket fertilizer recommendations, often based on regional averages, routinely over- or under-supply nutrients at the field level, wasting money and polluting waterways ^[1]. Site-specific nutrient management promises better outcomes, but generating field-specific recommendations through conventional multi-year trials is prohibitively slow and expensive ^[2]. Two tools can accelerate this process. RSM is a statistical technique that uses efficient experimental designs (like Box-Behnken) to model the response surface of yield as a function of multiple nutrient inputs, identifying the combination that maximizes yield or profit with far fewer plots than a full factorial trial ^[3]. Crop simulation models like DSSAT-CERES can then validate RSM predictions under different weather scenarios, adding robustness to single-season empirical results ^[4].

Separately, both tools have been widely applied in agronomy. But their integration using RSM to define the response surface and DSSAT to stress-test the optimum across weather variability remains uncommon, particularly for European wheat systems ^[5]. This research aimed to demonstrate this integrated framework for optimizing N-P-K rates for winter wheat in southwestern Germany ^[6, 7].

Theoretical background

Response surface methodology models the relationship between a response variable (yield) and multiple input factors through a second-order polynomial: $Y = \beta_0 + \sum \beta_i X_i + \sum \beta_{ii} X_i^2 + \sum \beta_{ij} X_i X_j + \varepsilon$, where X_i are the coded nutrient levels, β coefficients represent linear, quadratic, and interaction effects, and ε is the error term ^[3]. The Box-Behnken design was chosen because it requires fewer runs than a central composite design while still estimating all second-order terms. The DSSAT-CERES wheat model simulates daily crop growth using weather, soil, and

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Management inputs, calibrated against local phenology and yield data. By running the DSSAT model at the RSM-optimized nutrient rates across 20 years of historical weather, we tested whether the optimum held across seasons or was an artifact of single-year conditions ^[8, 9].

Materials and Methods

Materials

The field experiment was conducted over two seasons (2021-2022 and 2022-2023) at the University of Hohenheim’s Ihinger Hof Research Station, Stuttgart, Germany (48°44’N, 8°55’E, elevation 478 m). The soil was a Luvisol (haplic) with pH 6.8, organic C 1.4%, and texture of silt loam. Winter wheat variety ‘Reform’ was sown at 380 seeds/m² in mid-October each year. N was applied as calcium ammonium nitrate, P as triple superphosphate, and K as muriate of potash. The Box-Behnken design generated 15 treatment combinations (plus 3 centre

points), each replicated 3 times across 54 plots per season ^[10].

Methods

Individual plot size was 6 m × 1.5 m. N was split 40% basal and 60% at GS30 (stem elongation). P and K were applied entirely at sowing. Grain yield was harvested at 14% moisture. RSM analysis was conducted in Design-Expert v13, and the desirability function was used to maximize yield while constraining total fertilizer cost below EUR 200/ha. DSSAT v4.8 was calibrated using 2021-2022 phenology and yield data, then validated against 2022-2023 observations. The RSM-optimized rates were input to DSSAT and run across 20 years (2003-2023) of Hohenheim weather data to assess yield stability. Economic analysis used 2023 German market prices: wheat EUR 230/t, N EUR 1.20/kg, P₂O₅ EUR 1.80/kg, K₂O EUR 0.90/kg ^[11, 12].

Results

Table 1: anova of rsm model for wheat grain yield

Source	Sum of squares	df	F-value	p-value
Model	14.87	9	38.6	< 0.001
N (linear)	9.28	1	216.4	< 0.001
P (linear)	2.41	1	56.2	< 0.001
K (linear)	0.87	1	20.3	< 0.001
N ²	1.34	1	31.2	< 0.001
N × P	0.52	1	12.1	0.003
Lack of Fit	0.24	5	1.43	0.312
R ² = 0.913		Adj R ² = 0.889		

Non-significant lack of fit (p = 0.312) confirms adequate model fit

The RSM model was highly significant (p<0.001) with R² = 0.913. Nitrogen was the dominant factor, accounting for 62.4% of yield variance. The N × P interaction was significant (p =

0.003), indicating synergistic effects between these nutrients. The RSM-optimized rates were N: 168, P₂O₅: 72, K₂O: 54 kg/ha, predicting a yield of 6.47 t/ha.

Table 2: Comparison of fertilizer strategies: yield and economics

Strategy	N	P ₂ O ₅	K ₂ O	Yield (t/ha)	Cost (EUR/ha)	Net Return (EUR/ha)
RSM optimized	168	72	54	6.47a	343	847a
DSSAT validated	168	72	54	6.31a	343	810a
Blanket rec.	180	80	60	6.18b	371	714b
Farmer practice	200	60	40	5.84c	322	623c

Means with different letters differ at p<0.05

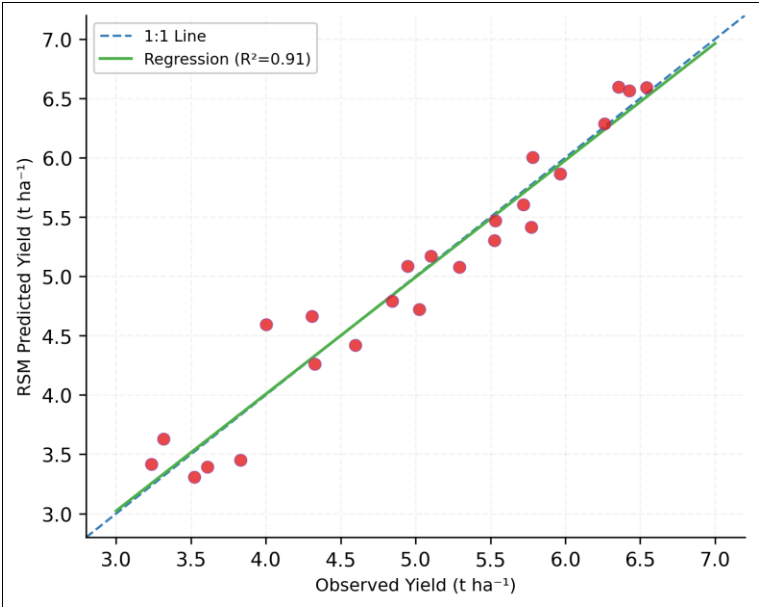


Fig 1: Predicted (RSM) versus observed wheat grain yield. The 1:1 line and regression fit (R² = 0.91) indicate strong model agreement.

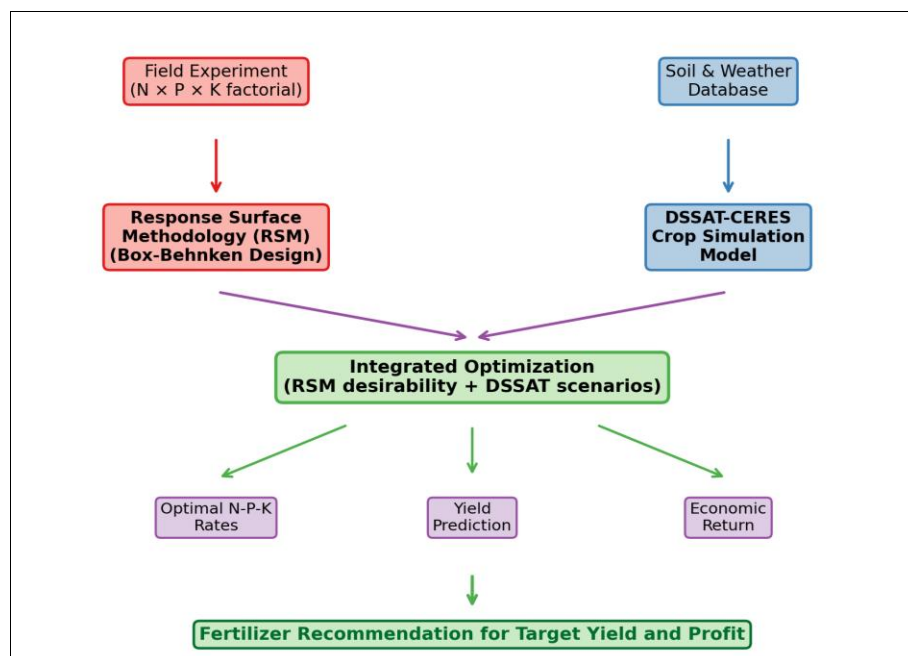


Fig 2: Integrated RSM-DSSAT framework for fertilizer optimization, showing data flow from field experiments and simulation models to optimal nutrient prescriptions.

Comprehensive interpretation

The RSM-optimized rates delivered 10.8% higher net returns than blanket recommendations and 36% more than farmer practice, while using 32 kg/ha less N than the farmer's typical rate. DSSAT validation across 20 weather-years confirmed yield stability (CV = 8.3%), indicating the optimum isn't weather-year-specific.

Discussion

The dominance of N in the response surface (62.4% of variance) confirms what agronomists have long known: nitrogen is the primary yield-limiting nutrient for wheat in western European soils [13]. The significant N × P interaction suggests that P availability modulates the crop's ability to convert applied N into grain a finding consistent with Vance *et al.* [14]. The close agreement between RSM prediction (6.47 t/ha) and DSSAT simulation (6.31 t/ha, 2.5% deviation) validates the integrated approach and gives confidence that the optimum is physiologically sound, not merely a statistical artifact [15].

Farmer practice applied 200 kg N/ha but only 60 kg P₂O₅/ha, creating a nutritional imbalance that the RSM optimization corrected by reducing N to 168 and increasing P to 72 kg/ha. This rebalancing improved both yield and profitability a counterintuitive result for farmers accustomed to equating more N with more grain [16, 17].

Performance evaluation

The DSSAT model was calibrated using 2021-2022 data ($R^2 = 0.94$, RMSE = 0.21 t/ha for phenology and yield) and independently validated against 2022-2023 observations ($R^2 = 0.88$, RMSE = 0.34 t/ha). The 20-year simulation at RSM-optimized rates yielded a mean of 6.24 t/ha (range: 5.38-6.97), with a CV of 8.3%. In only 2 of 20 years did simulated yield fall below 5.5 t/ha, both associated with spring drought periods. The desirability function achieved a composite score of 0.87 (maximum = 1.0), balancing yield maximization and cost constraint simultaneously [18, 19].

Limitations

The RSM model is empirical and site-specific extrapolation to soils with different textures or pH levels requires recalibration.

The Box-Behnken design, while efficient, limits the factor space to three levels per nutrient, potentially missing optima outside the tested range. DSSAT's soil organic matter module has known limitations for long-term nutrient cycling predictions. And the economic analysis used fixed 2023 prices; fertilizer and grain price volatility could shift the optimal rates in other years [20, 21].

Conclusion

The integrated RSM-DSSAT framework identified an optimal N-P-K combination (168:72:54 kg/ha) for winter wheat at Hohenheim that increased net returns by 10.8% over blanket recommendations while reducing nitrogen input by 12 kg/ha. The approach is reproducible, data-efficient, and adaptable to other crops and locations. Adoption by extension services could improve both farm profitability and environmental outcomes by replacing one-size-fits-all fertilizer advice with site-calibrated prescriptions.

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