3.7. Plant Critical N Concentrations and N Deficit Factors

Plant growth is greatly affected by the supply of N. Typically the supply of N to plants at the beginning of the season is often relatively high and becomes lower as the plant reaches maturity. The concentration of N in plant tissues also changes as the plant ages. During early growth, N concentrations are usually high due to synthesis of large amounts of organic N compounds required by the biochemical processes constituting photosynthesis and growth. As the plant ages, less of this new material is required and export from old tissues to new tissues occurs, lowering the whole plant N concentration. At any point in time there exists a critical N concentration in the plant tissue below which growth will be reduced.

Attempts to describe relationships between concentrations of nutrients in their tissues and rates of plant growth abound in the literature (see Olson and Kurtz, 1982 for a review). Most of the studies reported use either nutrient concentration in a specified plant organ (e.g., ear leaf in maize or flag leaf in wheat) or report a critical concentration at a specified age. Other studies (e.g., Greenwood, 1976) have correlated specific extracts of N from the tissues with plant growth. When attempting to model the continuous effect of a nutrient deficiency on plant growth from emergence to maturity, few of these critical concentration values reported for single organs at single times are of value. Others (e.g., Angus and Moncur, 1982) have attempted to overcome this by developing critical concentration curves as a function of time after planting. This approach has limited application for a model designed to simulate the growth of wheat crops with growth durations varying from less than 100 days in Canada and the tropics to over 250 days in Europe.

To provide generality, critical concentrations can be expressed as functions of plant age. Penning de Vries (1982) has described a stylized general relationship for the concentration of N as a function of plant age in C3 and C4 plants. Jones (1983) has developed this approach further by quantifying critical concentrations of N and P in maize and sorghum as a function of plant phenological age.

To develop appropriate relationships for critical N concentrations in wheat, published data from field experiments that met the following criteria were assembled:

1. Experiments had a series of N rates with sufficient range to define optimal or near-optimal growth patterns.
2. Experiments were considered to have been conducted under conditions where the potential effects of other interacting factors (e.g., heat stress, moisture stress, frost, supply of other nutrients, etc.) were minimized.
3. Plant tops N concentration was reported at several times during the growing season.
4. The growth stage or phenological age of the crop was reported for the times of plant sampling.

In some cases, critical concentrations were defined by the authors and where appropriate these were adopted. In two studies only one N rate was used but was described as being an optimal rate by the authors. Data were drawn from the following sources (Table 3.4) representing a diversity of wheat genotypes and wheat-growing environments.

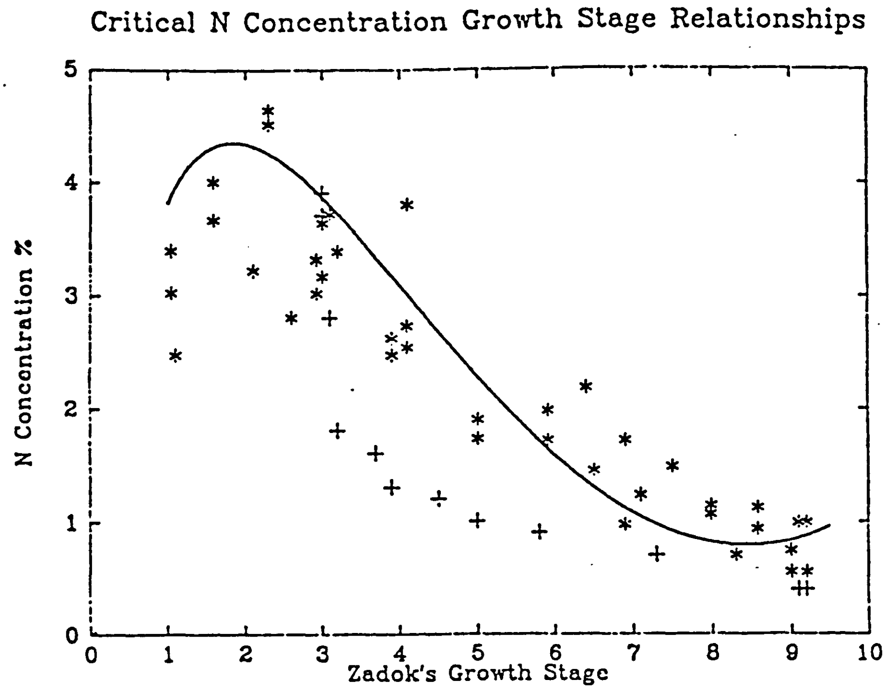
Table 3.4. Data Sources Used for Determination of Critical N Concentration Relationships

Author	Spring or Winter Wheat	Location
Engel and Zubriski (1982)	Spring	North Dakota
Campbell et al. (1977a)	Spring	Canada
Wagger et al. (1981)	Winter	Kansas
Leitch and Vaidanathan (1983)	Winter	U.K.
Wagger (1983)	Winter	Kansas
Waldren and Flowerday (1979)	Winter	Nebraska
Page et al. (1977)	Winter	U.K.
Alessi et al. (1979)	Spring	North Dakota
Mugwira and Bishnoi (1980)	Winter	Alabama
Boatwright and Haas (1961)	Spring	North Dakota
Gasser and Thorburn (1972)	Spring	U.K.
Bhargava and Motiramani (1967)	Spring	Australia
Walia et al. (1980)	Spring	India
McNeal et al. (1968)	Spring	Montana
Spratt and Gasser (1970)	Spring	U.K.

From these data, relationships defining critical N concentration as a function of Zadoks' growth stage were determined. The critical N concentration was defined as the N concentration in the plant tissues at optimal or near-optimal growth (as defined by biomass, yield or leaf area from the response data). The relationship thus determined is defined as the concentration above which no further increases in crop growth occur and below which some effect on a growth process will occur.

Winter wheats and spring wheats were found to have different relationships (Figure 3.7). These relationships for the tops critical N percentage (TCNP) appear in subroutine NFACTO as a function of Zadoks' growth stage (ZSTAGE).

(a) Winter Wheats.



(b) Spring Wheats.

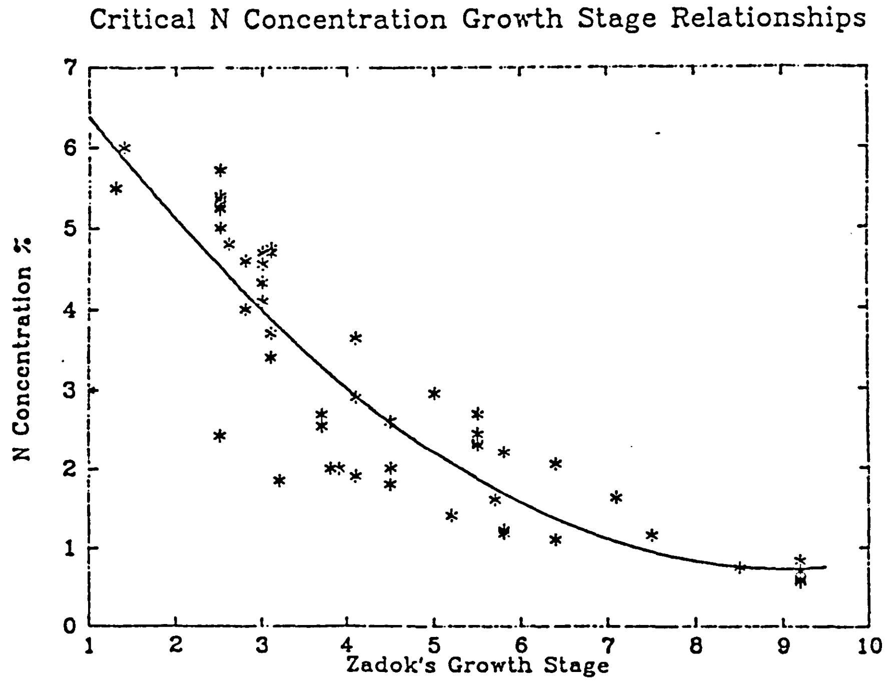


Figure 3.7. Observations Indicated by "+" Were Drawn From Page et al., (1977) and did not Fit Other Observations and Were Not Used to Fit the Function.

For winter wheats:

TCNP = -5.0112 - 6.3507 * ZSTAGE + 14.9578 * SQRT(ZSTAGE) + 0.2238 * (ZSTAGE * ZSTAGE)

For spring wheats:

TCNP = 7.4532 - 1.7908 * ZSTAGE + 0.6093 * SQRT(ZSTAGE) + 0.0934 * ZSTAGE * ZSTAGE

Root Critical N Concentration (RCNP) relationships were derived from the greenhouse data of Smith et al. (1983) and Day et al. (1985).

RCNP = 2.10 - 0.14 * SQRT(ZSTAGE)

The minimum concentration of N in plant tissues as a function of plant age is seldom reported. To formulate an appropriate relationship for use in the model, some of the lowest concentrations reported in the above studies were used as well as those reported from an extensive survey of N concentration in wheat crops spanning several years and locations in South Australia by Schultz and French (1976). In the model the tops minimum concentration (TMNC) is calculated as a function of model growth stage (XSTAGE):

TMNC = 2.97 - 0.455 * XSTAGE

Root critical minimum N concentration (RMNC) is used during the grain filling calculations (in subroutine GROSUB) and is assumed to be a constant 75% of the critical concentration.

RMNC = 0.75 * RCNP

The coupling of these functions to the phenology routines thus enables critical concentrations to be determined for any variety growing in any environment.

The critical and minimum concentrations are used to define a nitrogen factor (NFAC) which ranges from zero to slightly above unity. NFAC is the primary mechanism used within the model to determine the effect of N on plant growth. It is an index of deficiency relating the actual concentration (TANC) to these critical concentrations. NFAC has a value of zero when TANC is at its minimum value of TMNC and increases to 1.0 as concentration increases toward the critical concentration. It is calculated as:

$$NFAC = 1.0 - (TCNP - TANC)/(TCNP - TMNC)$$

Since all plant growth processes are not equally affected by N stress, a series of indices based on NFAC are used. For photosynthetic rate (NDEF1) and tillering (NDEF3), the indices are calculated as:

$$NDEF1 = NDEF3 = NFAC * NFAC$$

For leaf expansion growth (NDEF2) a less sensitive factor is used:

$$NDEF2 = NFAC$$

For the calculation of these indices NFAC has a maximum value of 1.0. This implies that when TANC exceeds TCNP no extra growth occurs.

A fourth factor used to modify the rate of grain N accumulation (NDEF4) is also calculated from NFAC, and can range from 0.0 to 1.5.

$$NDEF4 = NFAC * NFAC$$

These relations are depicted in Figure 3.8.

In the growth subroutine (GROSUB) the law of the minimum is extensively used to modify rates of plant growth. For each of the major functions (e.g., photosynthetic rate, leaf expansion rate, tiller number determination) the minimum of several zero to unity stress indices is used to modify a potential rate for the process.

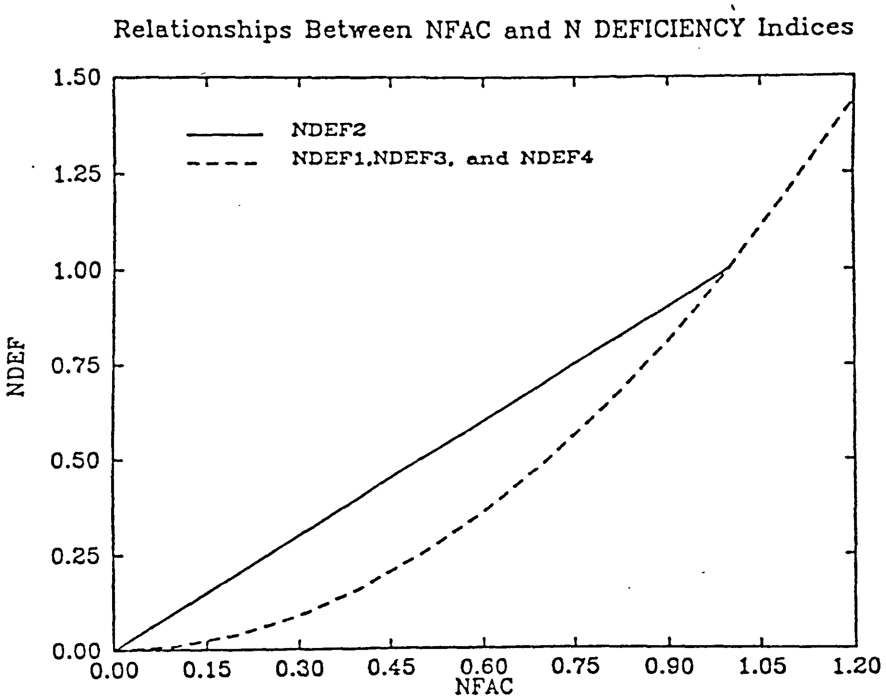


Figure 3.8. Relationship Between NFAC and the Nitrogen Deficit Factors (NDEF1, NDEF2, NDEF3, NDEF4). Only NDEF4 has Values Greater Than Unity.

3.8 Nitrogen Uptake

Plant roots may obtain nutrients from the soil by either interception of the nutrient in the soil by root growth, mass flow of the nutrient to the root associated with the flow of water, or by diffusion of the nutrient along a concentration gradient to the root surface (Barber, 1974). Mass flow and diffusion have been proposed and these are the subject of reviews by Barber (1974) and Barley (1970). Some of the comprehensive models (e.g., Hagin and Amberger, 1974; Zartman et al., 1976; Watts and Hanks, 1978) referred to earlier (Table 2.3) base N uptake calculations on a description of mass flow and diffusion of nitrate and ammonium in soil. These approaches do not consider the demand for the nutrient by the crop and consequently would have difficulty accurately describing N uptake for a young crop with low N demand when it is growing under conditions of high N supply. There have been differing approaches to combining the effects of soil supplying capacity and plant demand for nutrients. One of these (Claassen and Barber, 1976) uses functions describing mass flow and diffusion to predict a nutrient concentration at the root surface (C). Uptake is then estimated using a Michaelis-Menten function

$$I_n = \frac{I_{max}\ C}{K_m + C}$$

where,

I_n = net uptake.

I_{max} = the rate of uptake at infinite concentration.

K_m = the concentration when uptake is half of I_{max}.

I_{max} and K_m have been characterized for maize from solution culture experiments (Warncke and Barber, 1974) and field experiments (Mengel and Barber, 1974). I_{max} is an indicator of plant demand. This function has been used by Davidson et al., (1978a) and Selim and Iskandar (1981) in their comprehensive models. As an alternative to the Michaelis-Menten function, Nye and Tinker (1977) have proposed a single coefficient (α) termed "the root absorbing power". Wagenet et al., (1977) used this coefficient in their fertilizer transformation model. One problem that arises with the use of both these approaches to predicting uptake, is that plant demand changes with age. Edwards and Barber (1976) showed that I_{max} varied by an order of magnitude during the life cycle of the maize crop. A further problem with both α and I_{max} is that neither provide any capability for plant nutrient concentration to affect uptake. Novoa and Loomis (1981) cite evidence indicating that plant nitrogen concentrations can provide a negative feedback on nitrogen uptake rate.

The approach used in the CERES models has been to separately calculate the components of demand and supply and then use the lesser of these two to determine the actual rate of uptake. Demand can be considered as having two components. First there is a "deficiency demand." This is the amount of N required to restore the actual N concentration in the plant (TANC for tops) to the critical concentration (TCNP for tops). Critical concentrations for shoots and roots are defined in section 3.7. This deficiency demand can be quantified as the product of the existing biomass and the concentration difference as below:

TNDEM = TOPWT * (TCNP - TANC)

Similarly for roots the discrepancy in concentration (difference between RCNP and RANC) is multiplied by the root biomass (RTWT) to calculate the root N demand.

RNDEM = RTWT * (RCNP-RANC)

If luxury consumption of N has occurred such TANC is greater than TCNP then these demand components have negative values. If total N demand is negative then no uptake is performed on that day.

The second component of N demand is the demand for N by the new growth. Here the assumption is made that the plant would attempt to maintain a critical N concentration in the newly formed tissues. To calculate the new growth demand a potential amount of new growth is first estimated in the GROSUB subroutine. New growth is estimated from potential photosynthesis (PCARB) and is partitioned into a potential root growth (PGRORT) and a potential tops growth (PDWI).

Partitioning between potential shoot and root growth occurs as a function of plant phenological age:

PGRORT = PCARB * (60 - XSTAGE * 8)/100.

PDWI = PCARB - PGRORT

These potential growth increments provide a mechanism for the tops actual N concentration (TANC) to exceed TCNP. This occurs when some stress prevails and the actual growth increment is less than the potential. New growth demand for tops (DNG) is calculated as

DNG = PDWI * TCNP

and the new growth demand for roots is calculated as

PGRORT * RCNP.

During the early stages of plant growth the new growth component of N demand will be a large proportion of the total demand. As the crop biomass increases the deficiency demand becomes the larger component. During grain filling, the N required by the grain is removed from the vegetative and root pools to form a grain N pool. The resultant lowering of concentration in these pools may lead to increased demand.

The total plant N demand (NDEM) is the sum of all of these demand components. Calculations of soil supply of N are on a per hectare basis, which necessitates recalculation of the per plant demand into a per hectare demand (ANDEM).

ANDEM = NDEM * PLANTS * 10.0

To calculate the potential supply of N to the crop, zero to unity availability factors for each of nitrate (FNO3) and ammonium (FNH4) are calculated from the soil concentrations of the respective ions:

FNO3 = 1.0 - EXP(-0.0275 * NO3)L))

FNH4 = 1.0 - EXP(-0.025 * NH4(L))

The coefficients used in these two functions, obtained by trial and error, were found to be appropriate over a range of data sets. The greater mobility of nitrate ions in soil is reflected by the larger coefficient (0.0275) in these equations.

A zero to unity soil water factor (SMDFR) which reduces potential uptake is calculated as a function of the relative availability of soil water:

SMDFR = (SW(L) - LL(L))/ESW(L)

To account for increased anaerobiosis and declining root function at moisture contents above the drained upper limit, SMDFR is reduced as saturation is approached:

IF(SW(L) · GT · DUL(L))SMDFR = 1.0 - (SW(L) - DUL(L))/(SAT(L) - DUL(L))

The maximum potential N uptake from a layer may be calculated as a function of the maximum uptake per unit length of root and the total amount of root present in the layer. The first of these is a temporary variable (RFAC) which integrates the effects of root length density (RLV(L)), the soil water factor described above, and the depth of the layer:

RFAC = RLV(L) * SMDFR * SMDRF * DLAYR(L) * 100.0

The second of these equations incorporates the ion concentration effect (FNO3) and the maximum uptake per unit length of root (0.006 kg N/ha cm root) to yield a potential uptake of nitrate from the layer (RNO3U(L)).

RNO3U(L) = RFAC * FNO3 * 0.006

$RNO_3U(L)$ is thus the potential uptake of nitrate from layer L in kg N/ha constrained by the availability of water, the root length density and the concentration of nitrate. Initial estimates for the maximum uptake per unit length of root coefficient were obtained from the maize root data of Warncke and Barber (1974). This estimate was the subject of continuing modification during early model development. The value reported here appears to be appropriate across a broad range of data sets. The effect of each of these parameters on determining potential uptake can be seen in Figure 3.9. A similar function is employed to calculate the potential uptake of ammonium (RNH4U(L)).

```
RNH4U(L) = RFAC * FNH4 * 0.006
```

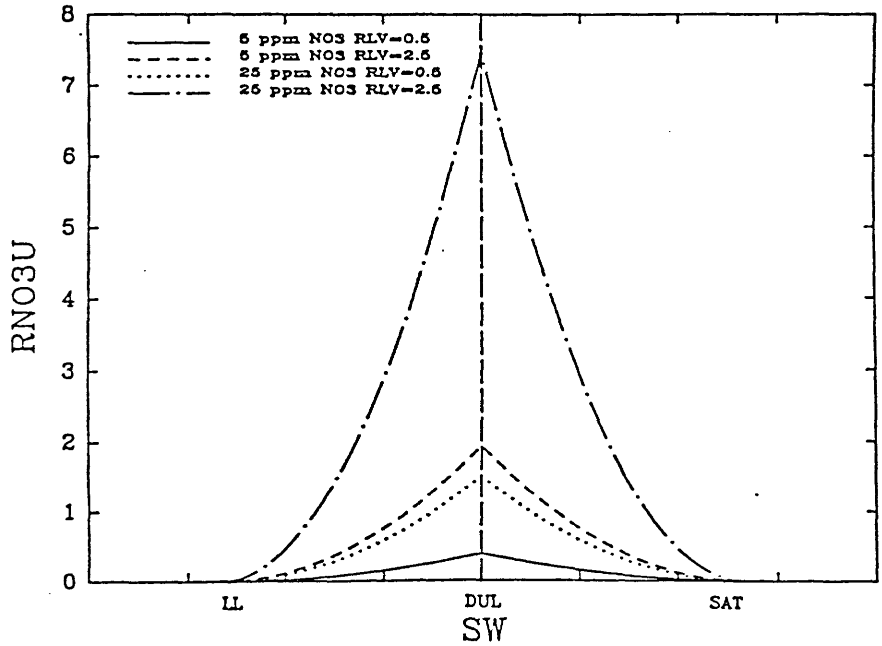


Figure 3.9. Simulated Effect of Changing Soil Water Status (SW on Potential Uptake of Nitrate From a Layer (RNO3U). LL, DUL, SAT Refer to the Lower Limit, Drained Upper Limit and Saturation Moisture Contents. The Four Curves Refer to Differing Concentrations of Nitrate (ppm NO_3) and Differing Root Length Densities (RLV in cm Root per Cubic cm of Soil).

To account for declining root function with increasing plant age during grain filling a term to reduce RFAC is introduced.

```
IF(XSTAGE · GT · 5.0)RFAC = RFAC * (6.0 - XSTAGE)
```

Potential N uptake from the whole profile (TRNU) is the sum of RNO3U(L) and RNH4U(L) from all soil layers where roots occur. Thus TRNU represents an integrated value which is sensitive to (a) rooting density, (b) the concentration of the two ionic species, and (c) their ease of extraction as a function of the soil water status of the different layers. This method of determining potential uptake enables the common condition, where N is concentrated in the upper layers of the profile, where most of the roots are present and where a nutritional drought due to shortage of water in these upper layers may occur, to be simulated. This can occur when the crop's demand for water is satisfied from soil water located deeper in the profile, but where there may be little N present.

If the potential N supply from the whole profile (TRNU) is greater than the crop N demand (ANDEM), an N uptake factor (NUF) is calculated and used to reduce the N uptake from each layer to the level of demand.

$$NUF = ANDEM/TRNU$$

This could occur when plants are young and have a high N supply. If the demand is greater than the supply then NUF has a value of 1.0. When NUF is less than 1.0 uptake from each layer is reduced as follows:

$$UNO3 = RNO3U(L) * NUF$$

$$UNH4 = RNH4U(L) * NUF$$

Following these calculations the soil mineral N pools can be updated for the actual uptake which has occurred.

$$SNO3(L) = SNO3(L) - UNO3$$

$$SNH4(L) = SNH4(L) - UNH4$$

Under conditions of luxury N uptake (TANC > TCNP) exudation of organic N compounds can occur. Rovira (1969) found changes in the shoot environment which cause more rapid growth can increase exudation, and Bowen (1969) reported that N deficiency can cause it to decrease. In the CERES-WHEAT-N model this exuded N is added to the fresh organic N pool (FON(L)) and can be mineralized and subsequently made available to the plant again. The amount of N which can be lost from the plant in this manner is calculated as 5% of the N contained in the roots/day. These losses are distributed to the FON(L)) pool according to the differing root length densities present in each layer as a proportion of the total root length.

IF(TANC · GT · TCNP)RNLOSS = RANC * RTWT * 0.05 * PLANTS *
RLV(L)/TRLV

Following uptake, concentrations of N in each of the shoots and roots are updated. To do this TRNU is converted from kg N/ha to a g N/plant basis.

TRNU = TRNU/(PLANTS * 10.0)

The proportion of the total plant demand (NDEM) arising from shoots (TNDEM) and roots (RNDEM) and the total root N loss (TRNLOS) are used to calculate the changes in N content of the shoots (DTOPSN) and roots (DROOTN).

DTOPSN = TNDEM/NDEM * TRNU - PTF * TRNLOS/(PLANTS * 10.0)

DROOTN = RNDEM/NDEM * TRNU - (1.0 - PTF) * TRNLOS/(PLANTS * 10.0)

TRNLOS is distributed over shoots and roots according to the plant top fraction (PTF) and must also be converted from a unit area basis to a per plant basis. Shoot and root N pools (TOPSN and ROOTN, respectively) can then be updated and new concentrations calculated:

TOPSN = TOPSN + DTOPSN

ROOTN = ROOTN + DROOTN

TANC = TOPSN/TOPWT

RANC = ROOTN/(RTWT + 0.5 * GRORT - 0.01 * RTWT)

When updating the root concentration allowance is made for the losses in root biomass occurring due to root exudation.

3.9. Crop Growth

N deficiency affects crop growth and yield primarily by affecting leaf area development, tillering, photosynthetic rate, and the partitioning of assimilate between plant parts. The growth routine of the CERES models simulates these processes and determines grain yield as the product of the simulated number of grains filled and their average weight. The method used to simulate each process is to estimate a potential rate for the process and then determine an actual rate by reducing this potential with a series of scalars describing the prevailing stresses. In each case the most limiting stress is used to determine the actual rate of the process. Temperature, soil-water deficit, and nitrogen deficiency stresses are each scaled on a zero to unity basis to facilitate the rate reduction calculations. Extensive documentation of the growth routine can be found in Ritchie et al. (1987). Only a brief summary highlighting the points where N deficiency effects are manifest is presented here.

Biomass production in the CERES models is simulated as a function of the amount of photosynthetically active radiation (PAR) which is intercepted by the crop. Solar radiation in units of MJ/m^2 is an input variable and PAR is calculated as a fraction of this. Interception is estimated as a function of the leaf area index of the crop (LAI).

From these relations, a potential biomass production PCARB (in units of g dry weight per m^2) is determined. A zero to unity temperature index (PRFT) is calculated from a weighted mean daily temperature. PRFT and the indices for soil and water deficit (SWDF1) and nitrogen deficiency (NDEF1) are used to reduce PCARB to an actual biomass production (CARBO) by the equation.

$$\text{CARBO} = \text{PCARB} * \min(\text{SWDEF1}, \text{NDEF1}) * \text{PRFT}$$

Respiration rates are assumed to be proportional to gross photosynthesis and are not calculated independently, but are incorporated into the calculation of PCARB and PRFT. The derivation of NDEF1 and the other stress indices are described in Section 3.7.

This same approach of using the most limiting factor to modify a potential rate of a process is used in the simulation of each of the major growth processes. These processes and the stress factors considered are tabulated below (Table 3.5). CARBO is partitioned into the various pools (leaf, stem, ear, grain, and root) dependent on the growth stage and prevailing stresses. Leaf area is developed by determining the potential rate of leaf expansion on the main stem and calculating leaf area for the whole plant by making an adjustment for tiller number. The simulated rate of tillering is affected by assimilate supply and the prevailing stresses. Grain number is estimated from stem size immediately prior to anthesis, and grain weight accumulation is simulated according to daily temperatures and the availability of assimilate from both photosynthesis and remobilization of material in stems and leaves.

From these relations, a potential biomass production PCARB (in units of g dry weight per m^2) is determined. A zero to unity temperature index (PRFT) is calculated from a weighted mean daily temperature. PRFT and the indices for soil and water deficit (SWDF1) and nitrogen deficiency (NDEF1) are used to reduce PCARB to an actual biomass production (CARBO) by the equation.

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Table 3.5. Stress Factors Used to Modify Plant Growth Processes in CERES-WHEAT

Plant Growth Process	Variable Names	Stage	Stress Factor Considered
Leaf expansion growth	PLAG	1	SWDF2, NDEF2, Temperature
Tillering	TILN	1	SWDF2, NDEF3, Tiller competition factor
Shoot/root partitioning	PTF	2,3,4	SWDF1, NDEF2
Tiller growth	TILSW	2,3	SWDF1, NDEF2
Senescence	CF, PLALR	1,2,3,4,5	SWDF1, NDEF4

3.10. N Redistribution During Grain Growth and Grain N Determination

In many wheat-growing areas, by the time the crop reaches the grain-filling stage, soil supplies of N are very low. In these cases the nitrogen requirement of the developing grains is largely satisfied by remobilization of protein from vegetative organs (Dalling et al., 1976, Simpson et al., 1983). These authors have shown this to be a complex process involving transport of nitrogenous compounds from the leaves to the roots and from the roots to the grain. When nitrogen supply is increased, the proportion of grain N arising from remobilization declines and the proportion from uptake increases (Vos, 1981). Many studies (e.g., Benzian et al., 1983, Terman et al., 1969) have found negative correlations between grain yield and grain protein concentration. Temperature and soil moisture also affect the grain nitrogen content. Constructing a model which captures most of these major effects has to date proved to be one of the most challenging tasks in the model development. Penning de Vries (1982) also concluded this to be a difficult task since many of the underlying concepts are often not clear and there are many unanswered questions.

When constructing the N grain-filling routines, procedures were adopted to closely mimic those predicting grain mass (or carbon) accumulation. In this procedure the rate of grain filling (RGFILL) (mg/day) is determined by temperature and thermal time (DTT).

$$\text{RGFILL} = 0.65 + (0.0787 - 0.00328 * (\text{TEMPMX} - \text{TEMPMN}) * (\text{TEMPM}-10.0) ** 0.8$$

where TEMPMX, TEMPMN, TEMPM are the maximum, minimum, and mean temperatures (°C), respectively. At mean temperatures of less than 10°C, RGFILL is linearly related to TEMPM

$$\text{RGFILL} = 0.065 * \text{TEMPM}$$

To determine the actual rate of grain filling for the whole plant (GROGRN), this rate is multiplied by a genetic factor (G3) supplied as input, and the number of grains per plant (GPP).

$$\text{GROGRN} = \text{RGFILL} * \text{GPP} * \text{G3} * 0.001$$

GROGRN is in units of g/plant/day.

To define similar functions for the rate of grain N accumulation (RGNFIL) (in micrograms per kernel per degree C day), the controlled environment studies of Sofield et al. (1977), Vos (1981) and Bhullar and Jenner (1985) were used. These studies examined various cultivars over a range of temperature conditions and other treatments. RGNFIL was found to be related to DTT (Figure 3.10) in these studies.

$$\text{RGNFIL} = 4.8297 - 3.2488 * \text{DTT} + 0.2503 *(\text{TEMPMX} - \text{TEMPMN}) + 4.3067 * \text{TEMPM}$$

and when the mean temperature is less than 10

$$\text{RGNFIL} = 0.483 * \text{TEMPM}$$

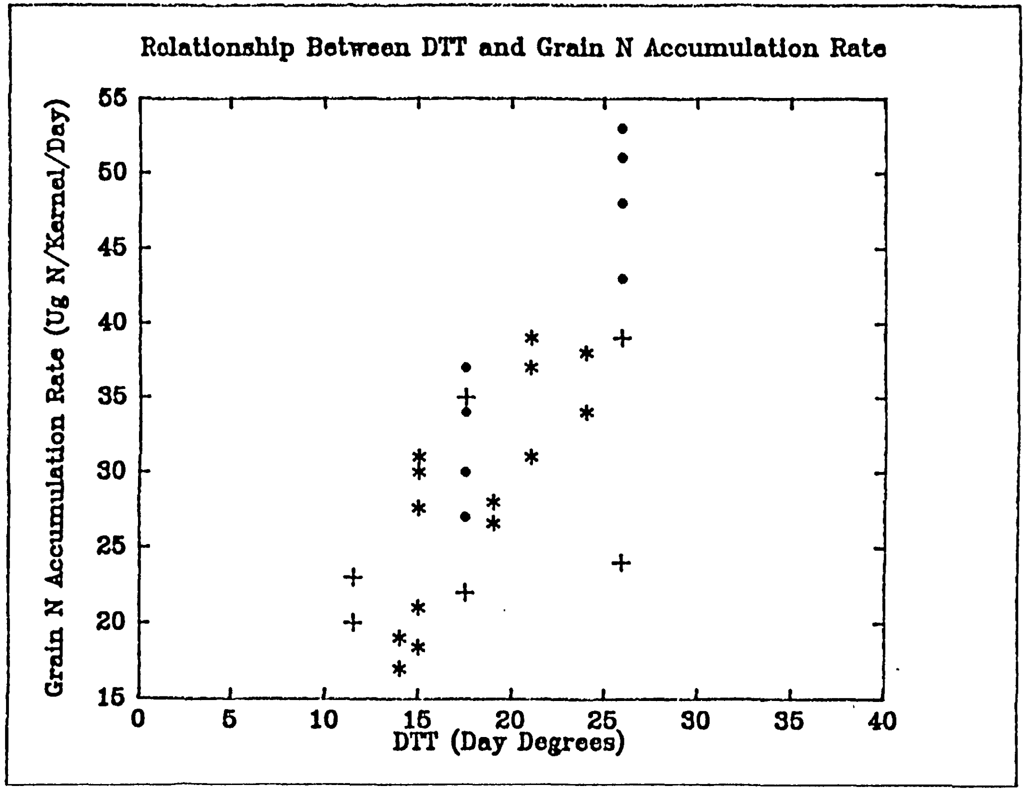

Figure 3.10. Relationship Between Calculated Daily Thermal Time (DTT) (Day Degrees) and the Rate of N Accumulation in Wheat Kernels (μg N/kernel/day). Data Were Drawn From Vos (1981), Safield et al., (1977), and Bhullar and Jenner (1985).

Maximum and minimum temperatures, while affecting the calculated value of DTT, can each affect RGNFILL differently (Figure 3.11) as indicated in the previous functions. A whole plant grain N sink (NSINK) can then be determined in similar manner to GROGRN.

NSINK = RGNFIL * GPP * 1.E-6 (g N/plant)

Since N stress will affect the rate at which plant tissues can mobilize N and supply it to the grain, an N stress factor NDEF4 from subroutine NFACTO is also introduced.

NSINK = NSINK * NDEF4

If N is present in the plant vegetative tissues (TANC greater than TCNP) the size of the sink is increased. If there is no grain N demand (NSINK = 0) on a day then no grain N accumulation occurs.

Two pools of N within the plant are available for translocation, a shoot pool (NPOOL1) and a root pool (NPOOL2). These pools are determined from the N concentration (VANC or RANC) relative to the critical concentration (VMNC or RMNC) and the biomass of the pool (RTWT or TOPWT).

NPOOL1 = TOPWT * (VANC-VMNC)

NPOOL2 = RTWT * (RANC-RMNC)

The total N available for translocation (NPOOL) is the sum of these two pools. When NPOOL is not sufficient to supply the grain N demand (NSINK), NSINK is reduced to NPOOL. If NSINK is greater than that which can be supplied by the tops (NPOOL1), then NPOOL1 is set to zero and the tops N concentration set to its minimum value (VMNC). The remaining NSINK is then satisfied from the root N pool and the root N pool updated accordingly.

NPOOL2 = NPOOL2 - (NSINK-NPOOL1)

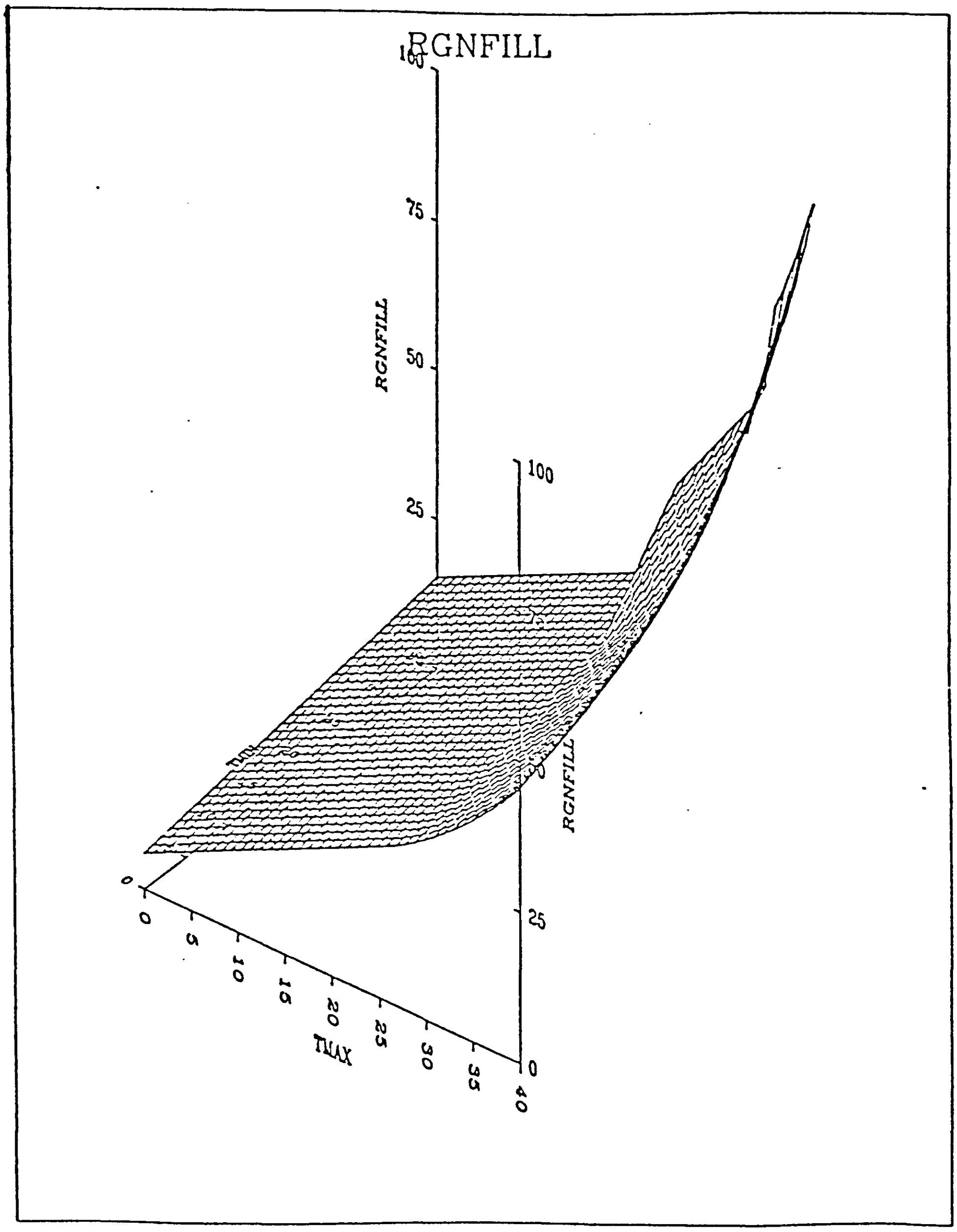

Figure 3.11. Effect of Maximum (TMAX) and Minimum (TMIN) Temperatures on the Simulated Rate of Grain N Accumulation (RGNFILL).

The root N concentration can then be updated.

RPOOLN = RTWT * RMNC + NPOOL2

RANC = ROOTN/RTWT

When NSINK is less than NPOOL1 it is totally satisfied from tops N

NPOOL1 = NPOOL1 - NSINK

and the tops concentrations updated accordingly.

TOPSN = NPOOL1 + VMNC * TOPWT

VANC = TOPSN/TOPWT

The total amount of N contained in the grain can then be accumulated

GRAINN = GRAINN + NSINK

This routine, together with the remainder of the growth routine and the N deficiency indices, thus can provide several pathways by which N stress during grain filling can affect grain yield and grain protein content. Firstly, as N is removed from the vegetative tissues NFAC will become lower. This will in turn lower NDEF4 and lower the sink size for N, thus providing for the capability of reduced grain N concentration. Lowering NFAC will also lower NDEF1 which will cause the rate of crop photosynthesis to fall, thus lowering the assimilate available for grain filling. A declining NFAC will also speed the rate of senescence which will reduce the leaf area available for photosynthesis. Different temperature regimes during grain filling will also affect the final grain N concentration since the function for RGNFIL is more sensitive to temperature than RGFILL. Soil water stress during grain filling can also increase the grain N concentration since SWDF1 will reduce photosynthesis, lowering assimilate availability and thus not diluting grain N as much as would occur in an unstressed crop.

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> "It is the mark of an instructed mind to rest satisfied with the degree of precision which the value of the subject permits and not to seek an exactness where only an approximation to the truth is possible."
>
> ----Aristotle

4.1. Validation Procedures

Before any model can be used with confidence, adequate validation or assessment of the magnitude of the errors that may result from their use should be performed. Model validation in its simplest form involves comparison between simulated values and real world values.

One measure of association between observed and predicted values often used is the correlation coefficient (r) or its square, the coefficient of determination (r^2). Willmott (1982) has pointed out that the main problem with this analysis is that the magnitudes of r and r^2 are not consistently related to the accuracy of prediction where accuracy is defined as the degree to which model predictions approach the magnitudes of their observed counterparts.

Dent and Blackie (1979) have proposed that model validation take the form of a simple regression analysis between mean model-outputs and real system measures as paired observations. As a result of the linear regression, a perfect model would provide a line passing through the origin with a slope of 1.0. They suggest testing the null hypothesis that the intercept coefficient (a) and the slope coefficient (b) simultaneously are not different from zero and unity, respectively. They have defined the F statistic to test this hypothesis as:

$$F = \frac{\{n-2\}\{n(a)^2 + 2n\bar{X}(a)(b-1) + \Sigma X_i^{\,2}(b-1)^2\}}{2n(S)^2} \qquad (4.1)$$

where X_i are the individual model-output values; $\bar{X}$ is the mean of model observations; and S is the standard error of the estimate.

The calculated value of F can then be compared with tabulated values at 2 and n-2 degrees of freedom.

The procedure can be further developed to determine which of the slope or intercept is in error. In this case a confidence interval about each of the slope and intercept coefficients can be formulated. Using the standard deviation Haan (1977) describes this procedure as follows:

$$L_\alpha = a - t_{1-\alpha/2,n-2}\ S_a \qquad (4.2)$$

$$U_\alpha = a + t_{1-\alpha/2,n-2}\ S_a \qquad (4.3)$$

for the intercept

and:

$$L_\beta = b - t_{1-\alpha/2,n-2}\ S_b \qquad (4.4)$$

$$U_\beta = b + t_{1-\alpha/2,n-2}\ S_b \qquad (4.5)$$

for the slope

where:

$n-2$ = degrees of freedom

$t_{1-\alpha/2}$ = 1-α/2 quantile of the Student's t distribution

L, U refer to upper and lower bounds, respectively, and

$$S_a = S^2\ [1/n + \bar{X}^2/\Sigma\ x_i^2]^{\frac{1}{2}}$$

$$S_b = S^2/(\Sigma\ x_i^2)^{\frac{1}{2}}$$

where S^2 = variances of the model prediction.

X_i, $\bar{X}$ as defined previously.

If the slope coefficient (b) is not within the bounds of the confidence interval (Ub and Lb), then the model has a consistent bias proportional to the magnitude of the observed data. If the intercept term (a) is not within the limits of the confidence interval (Ua and La) then the model has a consistent bias over the range of the observed data. Teng et al. (1980), Stapper (1984), and Otter-Nacke et al. (1986) have examined the a and b coefficients to effectively test models.

Willmott (1982) contends that further useful information on model performance can be gleaned from various difference measures. These measures are all dependent on the term $(P_i - 0_i)$ where P = predicted and 0 = observed. The measures reported by Willmott take the following form:

(1) Mean Bias Error (MBE)

$$\mathrm{MBE} = \sum_{i=1}^{n} (P_i - 0_i)/n \tag{4.6}$$

(2) Root Mean Square Error (RMSE)

$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{n} (P_i - 0_i)^2/n} \tag{4.7}$$

(3) Mean Absolute Error (MAE)

$$\mathrm{MAE} = \sum_{i=1}^{n} \left| P_i - 0_i \right| /n \tag{4.8}$$

The measures MAE and RMSE give estimates of the average error but provide no information on the relative size of the average difference between P and 0. MBE simply indicates the direction of the error. To overcome some of these shortcomings, Willmott has proposed an "index of agreement" d which has the form:

$$d = 1 - \left[\sum_{i=1}^{n} (P_i - O_i)^2 / \sum_{i=1}^{n} (\left| P_i' \right| + \left| O_i' \right|)^2 \right] \qquad (4.9)$$

where $P_i' = P_i - \bar{O}$ and $O_i' = O_i - \bar{O}$

The index is descriptive, but no criterion other than its relative magnitude (between 0 and 1) can be used to determine whether a model's performance is acceptable. The index is probably of value when comparing alternative models.

Wood and Cady (1984) have proposed the use of an "R test" for model validation. The test is appropriate when observed experimental data have been generated using either a completely randomized design or a randomized complete block design. The test uses comparisons of individual replicate data from each treatment against the simulated value for that treatment. Since the output of the simulation models has no variation due to replication, the same simulated value for a particular treatment is used in the comparisons with the individual observed replicate data from that treatment. The R value is used to test the null hypothesis that there is no difference between the simulated results and the treatment means. It has the form:

$$R_1 = \frac{\sum_{i=1}^{t} \sum_{j=1}^{r} (Y_{ij} - X_i)^2}{\sum_{i=1}^{t} \sum_{j=1}^{r} (Y_{ij} - \bar{Y}_i)^2} \qquad (4.10)$$

where:

Y_{ij} = observed yield from treatment i and replicate j (i = 1,...t and j = 1,...r)

$\bar{Y}_i$ = mean for treatment i

X_i = represents simulated yields from treatment i.

The null hypothesis for the above statistics is that there is no difference between the simulated result and treatment mean.

The test is appropriate where the assumptions for the F distribution (sums of squares criterion) are met and where individual replicate data are available. These assumptions are:

(i) the yield of the experiment must follow a normal distribution with variance ^{2} and the mean yield correctly specified by the model,

(ii) both the numerator and denominator must be multiples of chi-square random variables, and

(iii) the numerator and denominator have to be statistically independent. For most of the historical data used in the validation of the CERES model (Otter and Ritchie, 1985) and in this study, individual replicate data were not available and many of the experiments were not of these designs. Singh (1985) was able to employ this technique in an extensive validation of the CERES maize-N model using data from an international network of experiments.

An alternative approach to model validation has been suggested by Freese (1960). This measure enables the user to specify a degree of accuracy required (ε) and the level of probability for which predictions must be satisfactory (α). This may be formulated as:

$$P(\left|D\right| \leqq \varepsilon) \geqq 1 - \alpha \qquad (4.11)$$

where

$$D_i = O_i - P_i$$

and ε is in the same units as O. If the above criterion is met then the model is acceptable. If α is small then this requirement implies that the differences between predicted and observed values should be less than ε with high probability.

If D is normally distributed with $E(D) = 0$ then (5.11) will be satisfied provided

$$\varepsilon^2 \geqq \mathrm{Var}(D)\chi^2_{1-\alpha}(1),$$

where $\chi^2_{1-\alpha}(v)$ represents the 1-α quantile of the chi-squared distribution with v degrees of freedom. To test the acceptability of the model the null hypothesis below:

$$\text{Ho:} \quad E(D) = 0 \text{ and } \mathrm{Var}(D) \leqq \varepsilon^2/\chi^2_{1-\alpha}(1),$$

can be tested with the statistic:

$$\sum_{i=1}^{n} D_i^2/\mathrm{Var}(D) = \sum_{i=1}^{n} D_i^2\chi^2_{1-\alpha}(1)/\varepsilon^2$$

The null hypothesis can be rejected at significance level α' if the test statistic

$$\sum_{i=1}^{n} D_i^2\chi^2_{1-\alpha}(1)/\varepsilon^2 \qquad (4.12)$$

exceeds $\chi^2_{\alpha}{}^1(n)$.

The test will tend to reject Ho if Var(D) is large, or if E(D) is large, or if both these quantities are large so that it is sensitive to the two quantities that affect accuracy (Reynolds, 1984).

Reynolds (1984) has further modified the procedure to enable a critical error ε^* to be calculated. This critical error is given by:

$$\varepsilon^* = \left[\sum_{i=1}^{n} D_i^2 \chi^2_{1-\alpha}(1) / \chi^2_{1-\alpha}(n) \right]^{\frac{1}{2}} \qquad (4.13)$$

ε^* is the smallest value of ε which would lead to the rejection of the null hypothesis at the defined level of probability. The value of this approach is that it allows flexibility in testing models for users who may have different accuracy requirements.

Singh (1985) used this technique when examining the performance of the CERES-maize-N model. Using $\alpha = 5\%$ he found the critical error to be 1,200 kg/ha for grain yield across a range of data sets. The technique has also been used widely in forestry research (see Reynolds, 1984) for a review.

In the following analyses (section 4.3) model evaluation was undertaken by comparison of means and standard errors of observed and predicted data and the correlation between the observed and predicted pairs, as well as the procedures outlined by Dent and Blackie (1979), Wilmott (1982), and Reynolds (1984), depicted in equations 4.1 to 4.9 and equations 4.12 and 4.13.

The parameters examined in the statistical evaluation were:

1. Total above-ground biomass at harvest.
2. Grain yield.
3. N uptake in the above-ground plant parts at harvest.
4. N content of the grain.
5. Grain protein percentage.
6. Biomass of the crop at anthesis.
7. N uptake by the crop at anthesis.
8. Grains per square metre.
9. Weight of individual grains (mg).
10. Apparent recovery of fertilizer.

Comparisons were made using data from all the data sets listed where the observations were reported.

The ability of the model to simulate total nitrogen balance was tested with data from three contrasting data sets. In this analysis, observed values for soil mineral N (nitrate + ammonium) to the depth of observation were expressed in units of kilogram N per hectare and added to the observed values for plant N uptake. This provides an estimate of "accountable N." If, during the season, accountable N declines, then losses of mineral N from the soil/plant system must have occurred. If, during the season, accountable N increases, gains of N from net mineralization must have occurred. Comparison of observed accountable N with the corresponding simulated values thus tests the model's ability to simulate losses and accessions of N from the soil/plant system. The three data sets examined were Manhattan, Swift Current, and Lancelin (see following section). Each of the data sets had periodic plant harvests throughout the season with soil samples taken for analysis on the dates of harvest.

Statistical testing of a model has an aura of objectivity but considerable problems with interpretation can occur (Dent and Blackie, 1979). Grieg (1978) has advocated less "objective" approaches by using simple graphical display of model output in relation to the "controllable and uncontrollable exogenous variables and where possible relative to real system output." This form of model evaluation is of far greater value to the model builder than rigorous statistical testing since the nature and location of errors in model prediction are usually more readily detected. When certain errors are consistent across many data sets, then an alternative approach to modelling a particular process or subprocess which is known to occur at those locations can be adopted and the model reevaluated. Model evaluation thus is always an ongoing process.

Among the important objectives of development of the CERES-wheat-N model were to be able to:

1. Predict response or nonresponse to N fertilizer in a diversity of environments.
2. Predict crop N uptake and N utilization.
3. Substantially account for the N balance components in the soil-crop system.
4. Predict the time course of biomass accumulation and N uptake by the crop.

Due to differences in the nature of reporting individual data sets, statistical evaluation of each of these objectives for each data set would be difficult. These parameters are graphically depicted in this study where appropriate observed data were available.

4.2. Description of the Testing Data Base

Following the mode of testing of the CERES-wheat model (Otter and Ritchie, 1984), data sets of wheat production from several places in the world have been assembled for use in testing and improving the CERES-wheat model. Many of the data in the testing data base have come from published sources, many from unpublished Ph.D. theses, and some from other unpublished sources. In almost all cases a complete minimum data set was not available from the manuscripts and the additional climatic and soils information often had to be obtained from other reports or via personal communication. In some cases, where indicated below, when a few key data were not available, certain model inputs were estimated using the best available local information.

Since model development and testing is somewhat of an iterative process in the early stages, most of the data sets have been utilized during the development phase and are not truly independent. Since development of the N components of the model has necessarily lagged behind the development of the main model, the opportunity of rigorously testing the model with a large base of truly independent data sets has not yet arisen. Development and testing of the CERES-maize-N model (Jones and Kiniry, 1986) has proceeded in parallel with the work on the wheat model. Because the soil N transformation components of both models are identical and since the basic structure of the CERES-wheat model dictates the nature of biomass production, yield component determination, and water balance, the testing data base can be inferred as having some degree of independence from model development.

Thus, in the analyses that follow, no attempt has been made to separate truly independent data sets from those used for model development.

The test data base spans the range of wheat-growing environments from 53 degrees N latitude in the United Kingdom and the Netherlands with a 10-month growing season, to the spring wheat-growing areas of Canada and the northern United States with growing seasons of 90-120 days, to the winter planted spring wheat-growing areas of the middle east and Australia. A diversity of soil types and fertilizer application patterns, sources, and timings is also represented in the data base. A brief description of individual data sets follows.

(1) Garden City, Kansas, 1980

The experimental design was 6 N rates (0, 28, 56, 84, 112, and 140 kg N/ha) and four irrigation timing strategies (preplant irrigation only, preplant + irrigation at jointing, preplant + irrigation at flowering, irrigation at all three times). The experiment was performed on a clay loam (Aridic Argiustoll) soil. Fertilizers were all applied preplanting by broadcasting followed by incorporation. The variety was Newton. The experiment was conducted by Dr. Mark Hooker. Data were obtained by personal communication but are reported in Wagger (1983).

(2) Garden City, Kansas, 1981

The experimental design was identical to that described above. Data were obtained by personal communication from Dr. Hooker.

(3) Manhattan, Kansas, 1981

The experimental design consisted of three N rates and a plus and minus irrigation treatment. The three N rates were 0, 60, and 180 kg N/ha. The 180 kg N/ha rate was applied as 90 kg N/ha at planting and 90 kg N/ha 132 days after planting. Data are reported as Wagger (1983). Additional data were obtained by personal communication with Dr. M. Wagger and Dr. D. Kissel, Kansas State University.

(4) Hutchinson, Kansas, 1979 and 1980

The experimental design comprised 6 N rates 0, 28, 56, 84, 112, and 140 kg N/ha all applied preplanting followed by incorporation. In 1979 the variety used was Centurk and in 1980 Newton.

(5) Swift Current, Saskatchewan, Canada, 1975

The experiment is reported by Campbell et al. (1977a,b). The experiment comprised 7 N rates (0, 20.5, 41, 61.5, 82, 123, 164 kg N/ha) with a plus and a minus irrigation treatment. Following planting, 15 cm diameter lysimeters were driven into the soil to a depth of 120 cm. Five harvests during the growing season were made. The variety was Manitou. Climate and soils data were obtained from the authors. The instrument gathering solar radiation data malfunctioned for a 3-week period during the early grain filling stage. The missing data were estimated by fitting a function to radiation of maximum and minimum temperature, presence or absence of rainfall, and the day of the year. The reliability of these estimates is not known.

(6) Northwest Syria (ICARDA), 1979 and 1980

These experiments were conducted at four sites in Aleppo province in Syria by Dr. M. Stapper. At three of the sites, Brida, Jindiress, and Kafr Antoon, two N rates (0 and 60 kg N/ha) were used. At each of these sites three spring wheat varieties (Mexipak, Sonalika, and Novi Sad) were compared. At the fourth site additional irrigation treatments were added. At one site (Kafr Antoon) a late frost was suspected and on the Jindiress site the variety Mexipak suffered somewhat from rust (H. C. Harris, ICARDA personal communication). The data are reported by Stapper (1984).

(7) Wongan Hills, Western Australia, 1966

The experiment was reported by Mason and Rowley (1969). The experiment was designed to examine the fate of anhydrous ammonia and urea applied to a loamy sand. Since the model simulates both of these fertilizer materials as identical ammoniacal sources, comparisons were made with the mean of these two treatments. The experiment showed no significant differences between the sources. The rates of N applied were 0 and 61 kg N/ha applied preplanting. Solar radiation data were estimated from recorded hours of sunshine data. The variety was the spring wheat Gamenya.

(8) Lancelin, Western Australia, 1967

This experiment was performed on a very coarse, siliceous sand and was designed to examine the fate of urea applied at various intervals after planting. Urea at a rate of 77 kg N/ha was applied either at planting or at 2, 4, or 8 weeks after planting. Delaying the application resulted in an almost threefold increase in grain yield. Solar radiation for Perth 100 km distant was used as part of the climatic data set for this experiment. The experiment is reported by Mason et al. (1972).

(9) Rothamsted, England, 1975

The experiment was reported as Pearman et al. (1978) and involved the comparison of three varieties of winter wheat (Maris Huntsman, Capelle Desprez, and Maris Fundin) over eight rates of N (0, 30, 60, 90, 120, 150, 180, and 210 kg N/ha). The fertilizer was applied 163 days after planting. Few significant variety X N interactions were recorded. The initial soil mineral N values and soil water contents were interpolated from estimates provided by the authors.

(10) Flevopolder, Netherlands, 1975

The experiment was reported by Spiertz and Ellen (1978). The experiment was designed to test the effects of late applications of N on leaf area duration, assimilation nutrient uptake, and growth of grains. No zero N treatment was included, and thus, comparisons of apparent fertilizer recovery are not made. The soil in the experiment was a Maine clay in a reclaimed polder. A water table was present during the course of the growing season. This was simulated by assuming that layers in the profile below 1 m deep were filled to saturation. Without this assumption the model predicted considerable moisture stress. Soil mineral N analyses were made after the crop was planted, and thus, estimates based on these were used for the initial mineral N input values supplied to the model. The variety was the winter wheat variety, Lely.

(11) Wageningen, 1977

These data are reported by Ellen and Spiertz (1980). The experiment examined various strategies of splitting fertilizer applications on uptake and yield of grain. The variety used was the winter wheat Donata. The soil was reported as a river clay with 45% silt.

(12) Carrington, North Dakota, 1969-73

These data were reported by Bauer (1980). The experiments involved a comparison of several varieties of hard, red spring wheats over several rates of nitrogen and over 5 years. Half of the experiment was irrigated and the remainder dryland. Since this experiment yielded a massive data set, only selected contrasting years were utilized in the testing data base to avoid biasing the data base with too many points from one location. Straw yields and straw N percent were not reported in some instances and were estimated from the grain yields and grain protein concentrations using the regression procedures described in the publication. This may lead to some errors in estimation of observed biomass and N uptake.

(13) Wagga Wagga, N.S.W., Australia, 1962

These data were reported by Storrier (1966). The experiment utilized four rates of N. Half of the experiment was irrigated and the remainder dryland. As a split plot treatment a later application of 45 kg N/ha as sodium nitrate was made to half of the plots. Storrier reports a negative response to applied N, but examination of the variation in the experiment indicates more of a case of non-response to N. Some lodging was reported to have occurred in the high N plots which the model would not be able to account for. The initial mineral N in this experiment was very high. Several gaps existed in the weather record for this experiment. Solar radiation was estimated from hours of sunshine data, where possible from the recordings made either on the site or nearby. Where the record was blank for both sites, mean values for that time of year were used.

(14) Dufur, Pendleton, and Madras Oregon, 1971

These experiments were reported by Ambler (1974) and involved the comparison of five varieties of winter wheat over several different rates of fertilizer at several different sites in Oregon. Data from sites where climatic data were incomplete were rejected. The three remaining sites differ in annual rainfall and altitude. Solar radiation data from Klamath Falls were used for the Madras data set. Few significant variety x N interactions were recorded and so data from only two cultivars (Hyslop and Nugaines) were utilized. At Madras four rates of N (0, 90, 180, and 270 kg N/ha at planting) and a fifth treatment with 90 kg N/ha applied at planting with a second application of 90 kg N/ha applied at the booting stage were investigated. Initial levels of nitrate in the profile were high and the response to N was small. The experiment was irrigated. At the Dufur site, three rates of N (0, 17, and 34 kg N/ha) were used and at the Pendleton site four rates of N (0, 34, 67, and 101 kg N/ha) were used. No significant response to N was recorded at either site.

(15) Waite Institute, 1958

These data were reported by Barley and Naidu (1962). The experiment examined the response to N of two varieties (Gabo and Bencubbin). The rates of N used were 0, 33, 67, and 174 kg N/ha as ammonium sulfate. Solar radiation data were estimated from the recorded values of hours of sunshine. The soil was reported as a red-brown earth (Alfisol)

(16) Bozeman, Montana, 1977

These data were reported by Christianson and Killorn (1981). This experiment examined differences in fertilizer use efficiency for applications made at different times. Nitrogen was applied as ammonium nitrate after seeding or broadcast several hours prior to a sprinkler irrigation to simulate application of fertilizer through the sprinkler system. The study investigated the effects of four rates of N applied at planting (0, 50, 100, and 150 kg N/ha) and five split-application patterns with a total application rate of either 100 or 125 kg N/ha. The soil was a deep silt loam and N responses were very marked.

4.3. Validation: Difference Measures and Summary Statistics

4.3.1. Grain Yield

Simulated grain yields are tabulated against observed counterparts in Appendix 4.1. The means and standard error of predictions closely approached those of the observations (Table 4.1). The degree of scatter around the 1:1 line (Figure 4.1A) is very small. Thirty yield predictions from a total of 240 deviated more than one standard deviation from their observed counterparts. Data sets where predictions were poor, were those from Carrington, North Dakota (1969),

Table 4.1: Summary Measures for All Data Sets

Variable	Units	N	$\bar{O}$	$\bar{P}$	SO	SP	a	b	R	D	F
Biomass	kg/ha	222	10,313	11,719	3,375	3,897	189.3	1.118	0.82	0.86	15.907
Grain yield	kg/ha	240	3,953	4,227	1,716	1,719	145.6	1.033	0.84	0.91	3.263
Total N uptake	kg N/ha	223	110	121	47	45	7.0	1.042	0.72	0.83	7.8438
Grain N uptake	kg N/ha	215	84	87	34	31	4.4	0.996	0.74	0.85	1.298
Grain protein	%	215	12.3	11.7	2.95	3.55	0.198	0.939	0.55	0.74	2.933
Anthesis DW	kg/ha	161	7,254	8,681	2,166	2,818	261.7	1.161	0.58	0.70	22.771
Anthesis N uptake	kg N/ha	151	118	116	57.1	39.31	11.66	0.887	0.67	0.78	2.3370
GPSM	No.	152	12,381	11,861	4,668	5,324	362	0.929	0.63	0.78	1.080
Kernel weight	mg	134	33.6	37.9	7.02	8.40	0.998	1.096	0.34	0.59	18.69
App recovery	%	137	45.7	43.4	29.4	25.68	8.37	0.767	0.37	0.65	6.24
Accountable N*	kg/N/ha	184	87.0	87.9	54.9	59.0	2.37	0.983	0.85	0.92	0.04

Variable	Units	N	P	CISLOP	CIINT	χ^2	MAE	MBE	RMSE	RT	E*
Biomass	kg/ha	222	0	0.028	423.6	136.01	2,248.1	1,405.590	2,648.19	13.06	480.9
Grain yield	kg/ha	240	0.0400	0.030	173.9	85.08	806.08	274.43	1,024.16	15.39	186.5
Total N uptake	kg N/ha	223	0.0005	0.0392	6.34	133.03	28.55	11.535	36.27	22.43	65.9
Grain N uptake	kg N/ha	215	0.2752	0.0354	4.344	105.13	19.4	3.491	24.040	18.64	43.6
Grain protein	%	215	0.0554	0.0330	0.582	250.832	2.363	-0.550	3.192	18.65	5.8
Anthesis DW	kg/ha	161	0	0.0509	533.22	259.72	2,159.6	1,426.76	2,759.73	19.26	494.6
Anthesis N uptake	kg N/ha	151	0.1002	0.0467	8.239	82.46	34.36	-1.660	42.352	23.62	75.7
GPSM	No.	152	0.3422	0.0516	362.30	131.43	3,462.3	-520.78	4,355.36	22.43	778.6
Kernel weight	mg	140	0	0.0452	2.1724	274.77	8.091	4.2286	9.8738	12.00	17.6
App recovery	%	137	0.0026	0.0850	6.032	152.20	23.460	-2.281	31.177	69.48	55.5
Accountable N*	kg/N/ha	184	0.959	0.045	2.379	60.03	21.521	0.879	31.458	190.16	56.7

Note:
N = Number of observations.
$\bar{O}$ = Mean of observations.
$\bar{P}$ = Mean of predictions.
SO = Standard deviation of observations.
SP = Standard deviation of predictions.
a = Intercept term from regression of predicted on observed.
b = Slope term from regression of predicted on observed.
R = Regression coefficient.
D = Index of agreement (Willmott, 1982).
F = F statistic calculated as per Dent and Blackie (1979).
P = Probability of exceeding F.
CISLOP = 5% confidence interval about slope of regression line.
CIINT = 5% confidence interval about intercept of regression line.
χ^2 = Chi-square.
MAE = Mean absolute error (Willmott, 1982).
MBE = Mean bias error (Willmott, 1982).
RMSE = Root mean square error.
RT = Model accuracy (Freese, 1960).
E* = 5% critical error as defined by Reynolds (1984).
*Only for three data sets (see text).

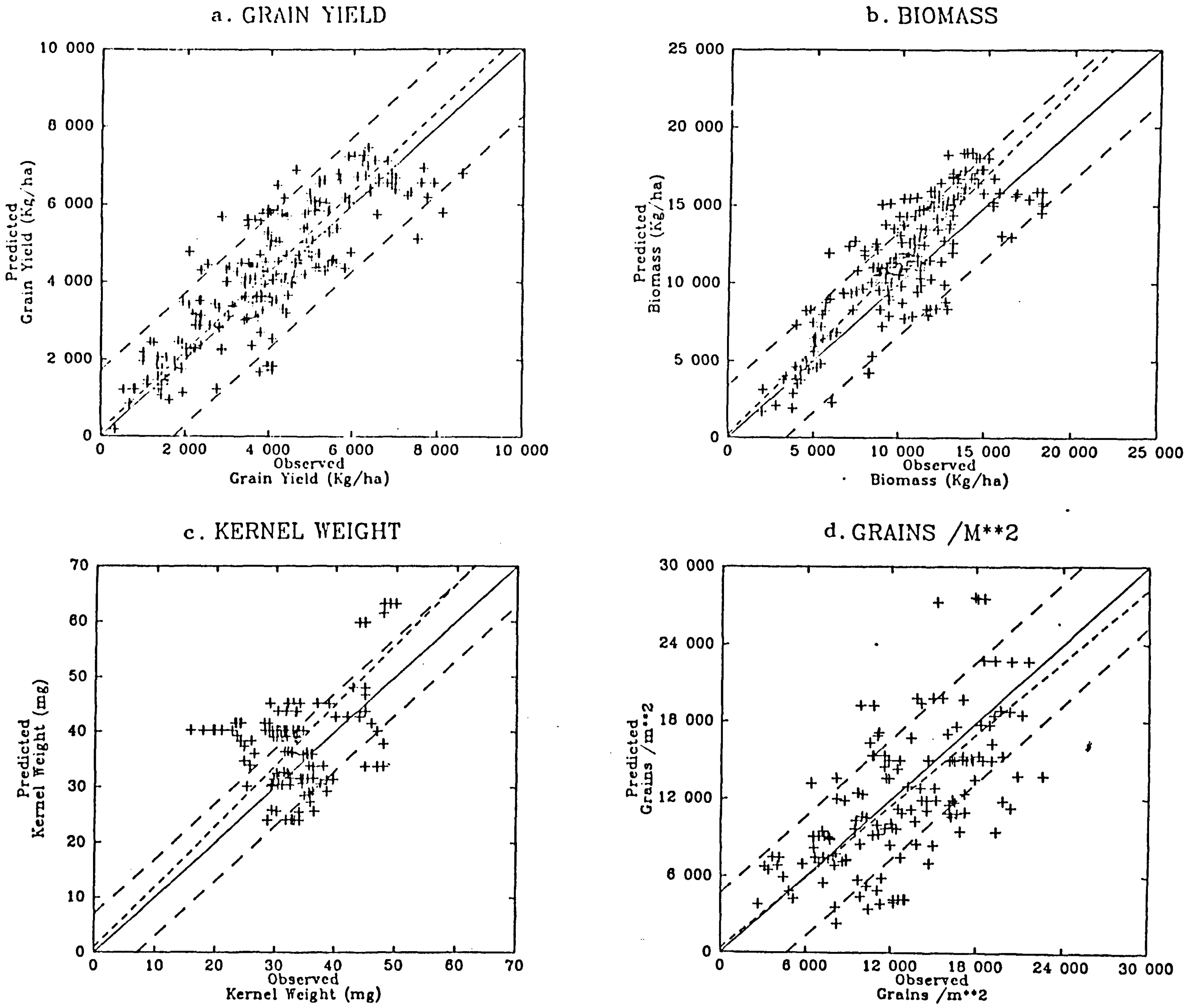


Figure 4.1. Comparison of Predictions of the CERES-WHEAT Model With Observed Data From Experiments.
In Each of the Figures ——— is the 1:1 Line.
----- is the regression Line Between Observed and Predicted.
— — — Mark the Boundary of ± 1 Standard Deviation From the Regression Line.

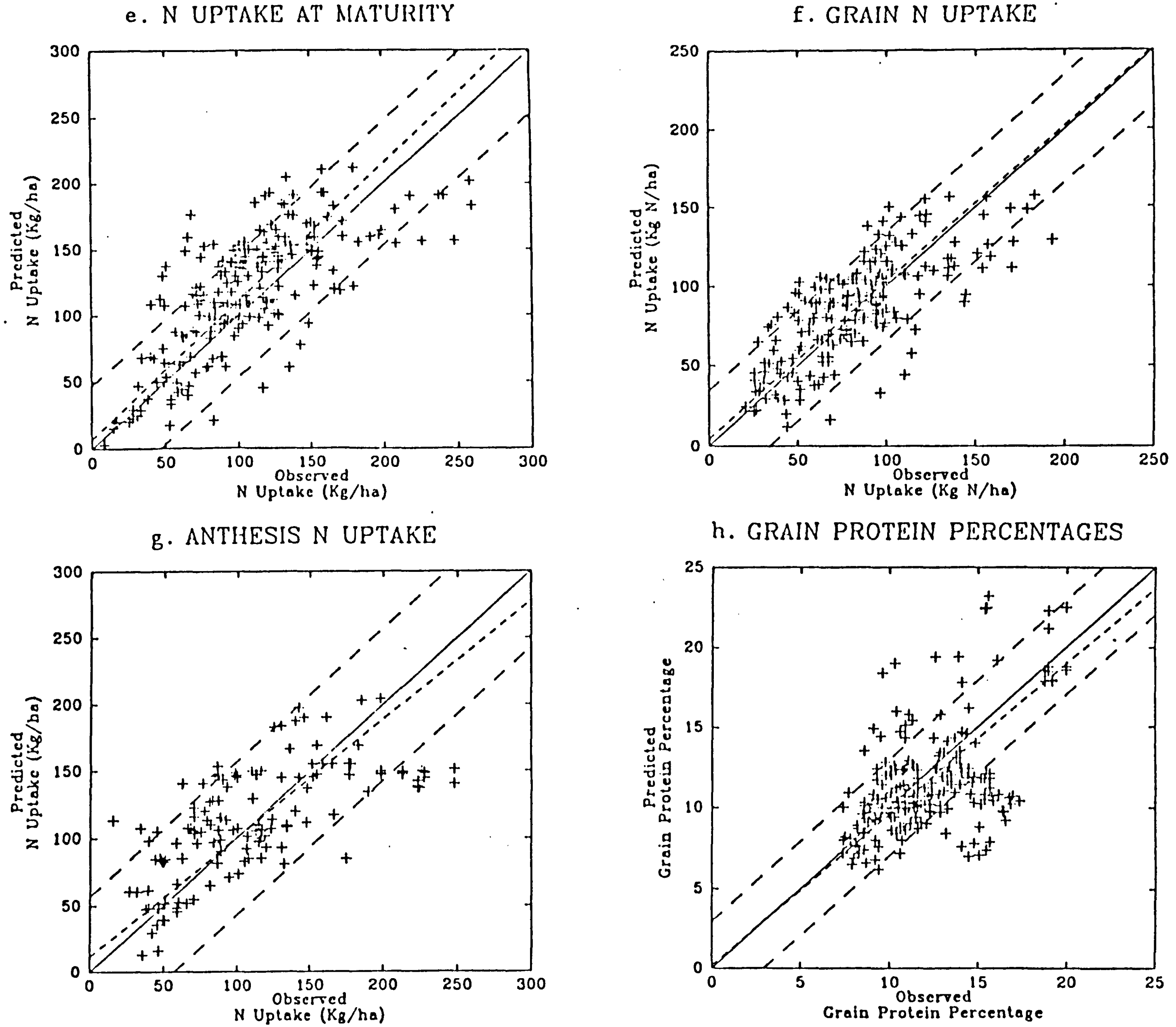


Figure 4.1. Continued.

Hutchinson, Kansas (1980), Flevopolder, Netherlands (1975), Jindiress, Syria (1980), and some individual treatments from some of the remaining data sets. The regression line (Figure 4.1A) has a slope greater than unity (1.033) which differs from unity by slightly more than 5% confidence interval (0.030). The F statistic for the regression is significant at the 5% level due to the slope. This slope of greater than unity and the small positive intercept (145.6 kg/ha) implies that the model has some tendency to overpredict yields across the range of observations. This is further indicated by the small positive MBE (Table 4.1). This is not surprising and certainly is insufficient to reject the model since the assumption is made that all nutrients other than N were present in nonlimiting quantities and that other factors not accounted for by the model (pests and diseases, crop lodging effects, frost induced sterility, etc.) had no influence on yield. As mentioned in the description of the data sets, these assumptions may not always have been entirely fulfilled. No quantitative data were available to suggest that some of the test data sets should have been eliminated from the testing data base.

All other statistical criteria for model evaluation (correlation coefficient, chi-square test, and modified Freese statistic) indicated the model was acceptable. The critical error term of Reynolds (1984) (Equation 4.13) indicates that the model will predict grain yield within an error of 1,865 kg/ha with a 95% confidence over the yield range observed (329 to 7,750 kg/ha).

4.3.2. Biomass

Simulated biomass is tabulated against its observed counterparts in Appendix 4.1. Means and standard error for predicted biomass closely resemble those from the observed data (Table 4.1). More scatter about the 1:1 line occurred for biomass predictions (Figure 4.1B) than for grain yield. The greater spread is in general due to a poorer simulation of straw yield. Most of the 55 points falling outside the bounds of the ±1.0 standard deviation were from whole data sets rather than from individual treatments across a range of data sets. Data sets where simulation of biomass was in general poor were: Wageningen, 1977; the variety Nugaines at Pendleton and Dufur, Oregon, 1971; various treatments within the Jindiress, 1980; Tel Hadya, 1980; Kafr Antoon, 1980; and Garden City, 1981. The simulated biomass for the Hutchinson 1980 data set was consistently low.

The slope of the regression line significantly deviated from the 1:1 line indicating a tendency of the model to overpredict biomass particularly at the high end of the range. This is also indicated by an MBE of 1,406 kg/ha. The correlation coefficient, chi-square and modified Freese statistic all indicated model predictions were acceptable.

4.3.3. Total N Uptake, Grain N Uptake, and Grain Protein

Performance of the model in predicting these parameters was in general poorer than the simulation for grain yield. Forty-four points from a total 223 fell outside the bounds of ±1.0 standard deviation of the 1:1 line for total N uptake, and for grain protein and grain N uptake this was 31 from 215 and 60 from 215, respectively. The slope of the regression line (1.042) for total N uptake was just beyond the 5% interval for slope (1.039). Similarly, the intercept (7.0) lies beyond the 5% confidence interval for the intercept (6.34).

There is a tendency for the simulations to exceed the observations although the correlation coefficient, chi-square test, and modified Freese procedure all indicate the simulations are acceptable. Total N uptake was consistently underpredicted for the Swift Current, Canada data and consistently overpredicted for the Waite Institute, Dufur, and Pendleton data sets.

Grain N uptake was simulated fairly closely (Figure 4.7). Much of the error involved in simulation of total N uptake arose from poor simulation of the concentration of N in the straw at harvest. The range of simulated values was consistently less than that observed (0.1%-1.3%). Some of these differences may occur due to differences in harvesting technique and time of harvest. If significant amounts of chaff or leaf material are not included in the sample, the reported straw N concentration will also be low. The model also makes no attempt to account for losses of N from the vegetative material through either leaching of N compounds from harvest ripe straw or via volatile losses from senescing leaves. Several of the data sets had less N in plant top tissue at harvest than at anthesis, indicating some losses occurred.

The scatter of points around the 1:1 line (Figure 4.1) was much higher for grain protein (grain N percent multiplied by 5.7 [Campbell et al., 1977b]) than for many other parameters. Both slope and intercept of the regression line are significantly different from the 1:1 line. The chi-square test also indicates the simulations are significantly different from the observations, but the modified Freese statistic indicates the model is still acceptable.

The simulation of grain protein concentration has been to date one of the most difficult components in the whole model to get working satisfactorily. In several of the data sets grain protein concentration was consistently overpredicted or underpredicted. It was difficult to determine if in any of these cases a genotypic factor was involved. Adding a further genetic coefficient to the model input data requirements to help explain cultivaral differences in grain protein accumulation has so far been avoided. Further investigation of this aspect of the model is warranted.

4.3.4. Dry Weight and N Uptake at Anthesis

In many of the studies harvests were made at or near anthesis. The simulated data used for the comparisons were the corresponding values for N uptake and biomass on the date of harvest (i.e., not necessarily on the simulated date of anthesis). Biomass was generally overestimated at anthesis. The regression line significantly deviates from the 1:1 line (Figure 4.1G) and 72 points of the 161 fell outside the bounds of ±1.0 standard deviation of the 1:1 line. The chi-square test indicated the predicted biomass differed significantly from that observed. The simulated N uptake at anthesis showed much less scatter than the predictions for biomass. The simulations were acceptable within all the statistical criteria examined. The model substantially underestimated the anthesis N uptake of several of the treatments from the experiments at Wagga Wagga, 1962. The resulting slope of the regression line thus is a little less than 1.0. Some compensating errors in the simulation of plant N concentration may occur if the simulated biomass is incorrect and the simulated N uptake is correct.

The MBE terms (Table 4.1) also indicate a large overestimate of biomass at anthesis and a slight underestimate of N uptake at anthesis.

4.3.5. Kernel Weight and Kernels Per Square Metre

Overall, the model had a slight tendency to underestimate the number of grains per square metre and overestimate the weight of individual kernels. The model consistently overestimated kernel weight for the variety Capelle Desprez in the Rothamsted 1975 experiments. In the determination of grain yield, some compensation can occur, such an overestimated kernel number is offset by an underprediction of kernel weights. These two yield components are, however, important indications to timing of certain stresses and, for the model to be useful, should be reasonably correct. For both parameters the slope of the regression line significantly differs from the 1:1 line but the intercepts were within the confidence interval. There was a noticeable tendency for the model not to display the same sensitivity in kernel weight to rates of applied N as the observed data did.

Some of the error in these two parameters may have been due to poor estimates of the genetic coefficients G2 and G3. (See Ritchie et al., 1987, for further details).

4.3.6. Apparent Recovery

Apparent recovery (AR) is a parameter often employed in fertilizer research to indicate the efficiency of fertilizer use. From a modelling standpoint it is a particularly challenging parameter on which to test the model since AR is dependent on the accurate simulation of two treatments simultaneously. It is calculated as below:

$$AR = \frac{NUP_f - NUP_u}{Rate} \times 100$$

where:

NUP_f = N uptake from a fertilized treatment

NUP_u = N uptake from an unfertilized treatment

Rate = rate of fertilizer applied.

Since AR depends upon the N uptake from two different treatments, small errors in the prediction of either can lead to quite spurious values for the calculated AR. This is indicated in Table 4.2 where 10% errors in prediction of both the fertilized and unfertilized treatment leads to errors in the calculated AR of 33% and 38%.

Table 4.2. Effect of Errors in N Uptake Simulation on Errors in Simulated Apparent Recovery

	NUP_f	NUP_u	Rate	AR	Error (%)
Sample Obs.	60	40	30	67	-
10% Error 1	66	36	30	100	33
10% Error 2	54	44	30	33	-34

The means and standard errors of the predictions closely approximated those of the observed. Most of the statistical parameters (Table 4.1) indicate a significant difference between predicted and observed values. The modified Freese 5% critical error value is 55. Viewed in the light of the problems of determination of AR and the magnitude of this critical value then the simulations should not be rejected.

4.4. Response to N in Individual Data Sets

The grain yield response to applied N in each of the individual data sets is plotted in Figure 4.2. Data sets where differing fertilizer strategies were examined are plotted separately (Figure 4.3). The Tel Hadya data set where irrigation strategies were examined is plotted separately (Figure 4.4) as well. In most instances the general pattern of grain yield response to N is well mimicked by the model. Some of the exceptions to this are noted below.

The model predicted no yield response to N or a very small positive response to N in each of the treatments from the Wagga Wagga 1982 experiment. The observed data tend to indicate a negative response to N but the predictions in all instances are within the bounds of the observed errors reported by Storrier (1965). Some lodging was also reported for this data set at the high rates of N which would have contributed to the seemingly negative response to N.

In the Hutchinson Kansas data sets the model overpredicts yield across the range of N rates in 1979 by approximately 30% and underpredicts yield by 55% across the range of N rates in 1980. Of all the data sets tested the model performed most poorly on this latter data set. The model simulated the Manhattan and Garden City data sets very reliably. These data sets had the same variety as the Hutchinson 1980 data set. The model was able to demonstrate sensitivity to both water regime and N supply in the Manhattan 1981 data set. Irrigation when no fertilizer was applied, caused a depression

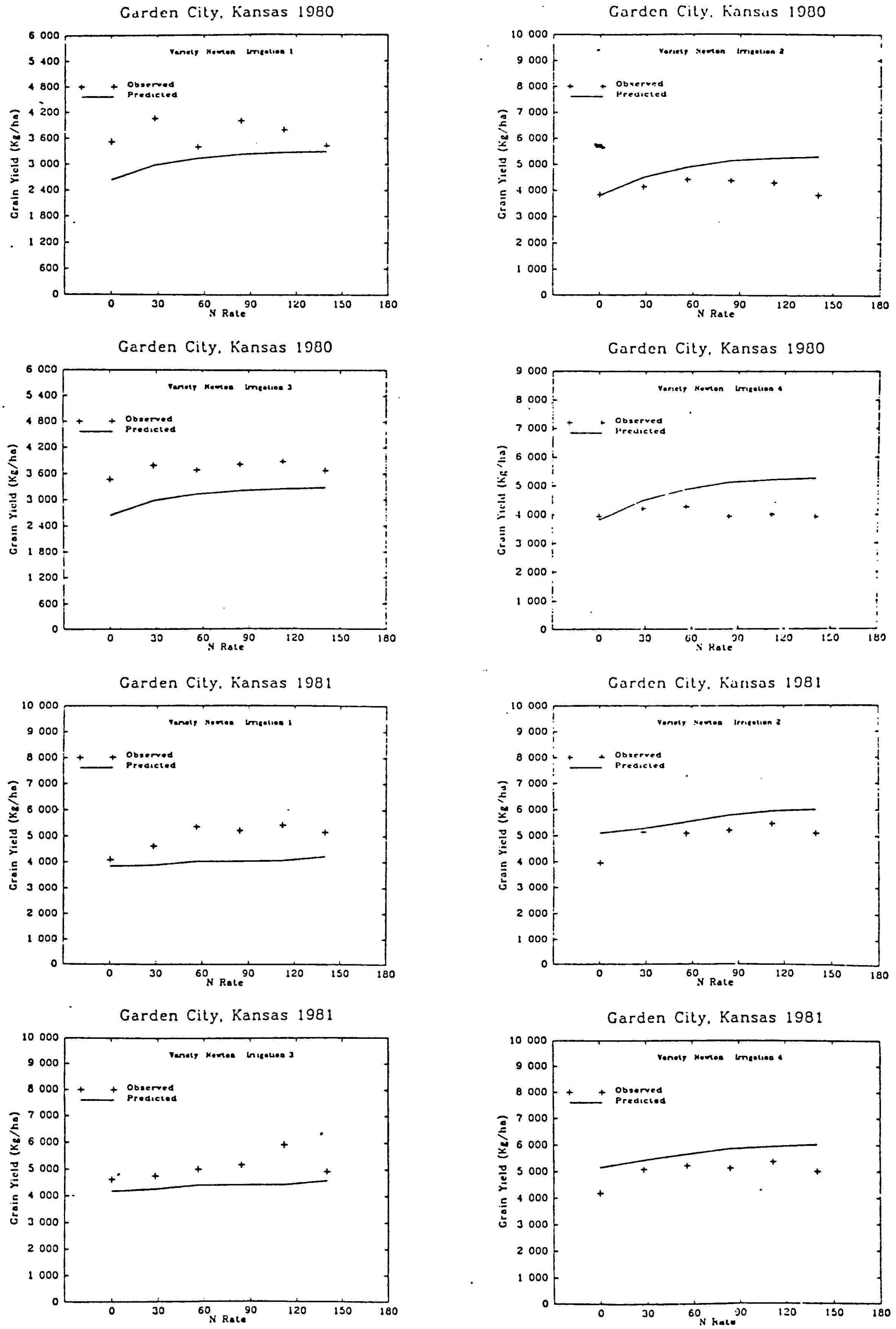
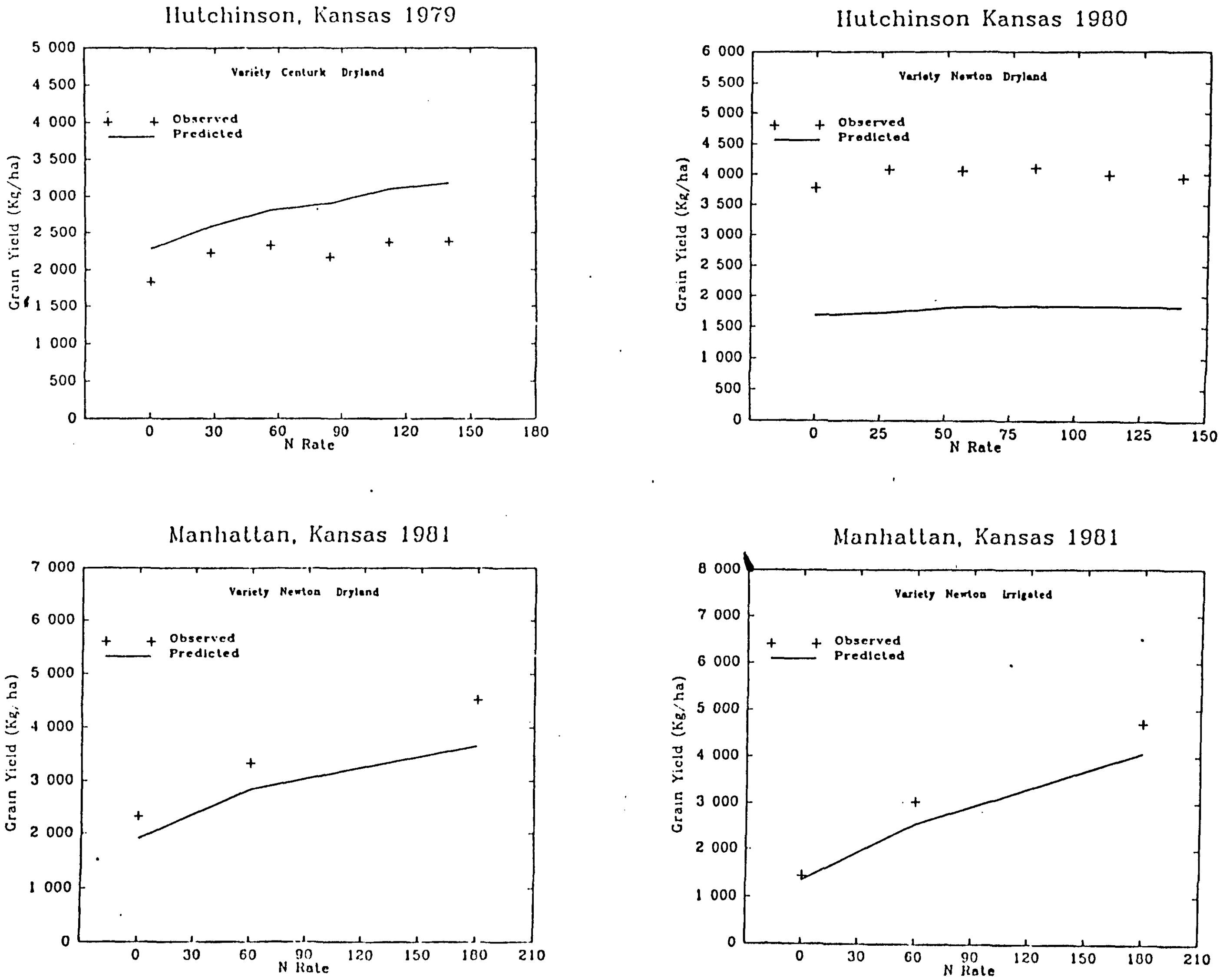


Figure 4.2. Comparison of Predicted and Observed Grain Yield Response to Applied N in Individual Data Sets.

Figure 4.2. Continued.



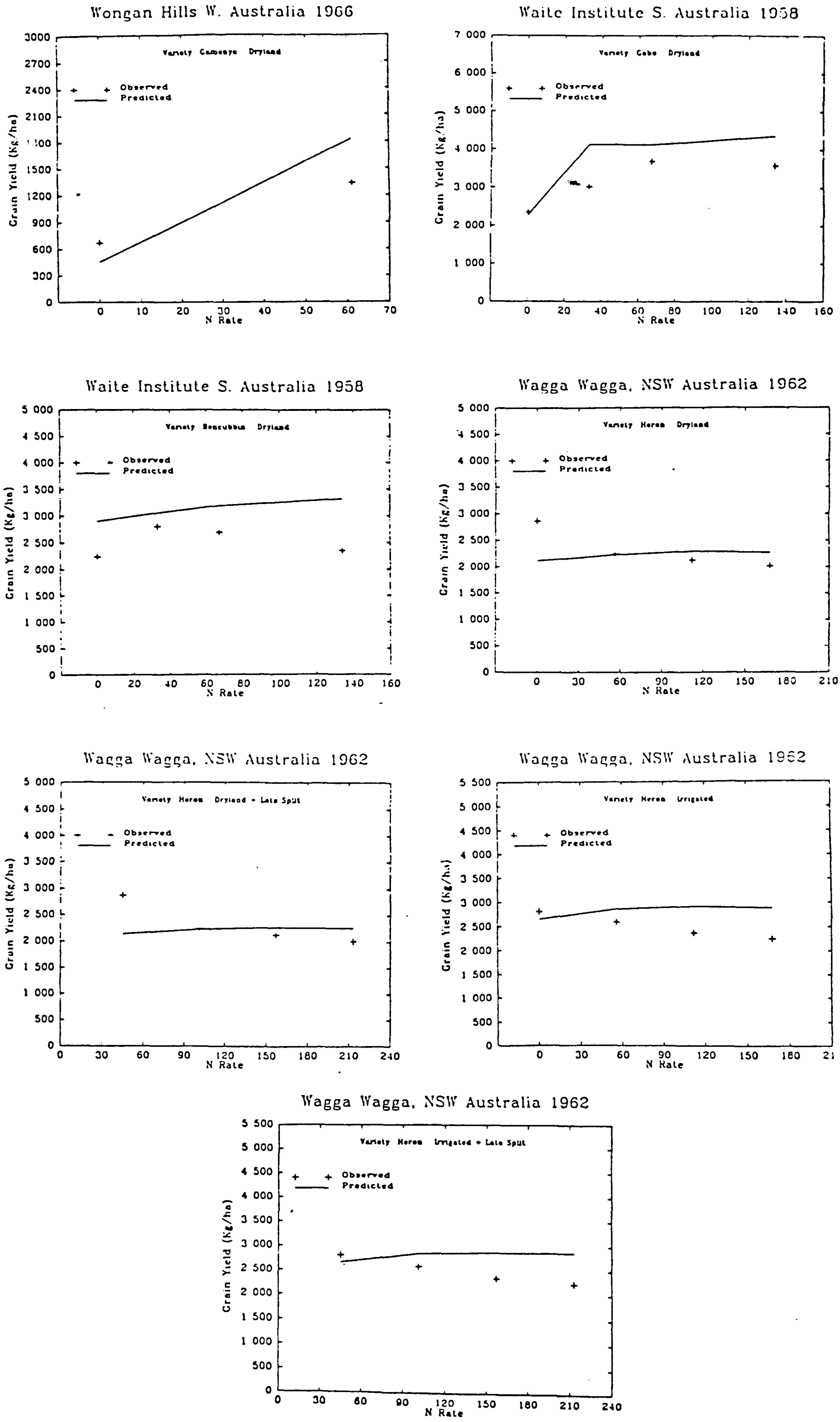


Figure 4.2. Continued.

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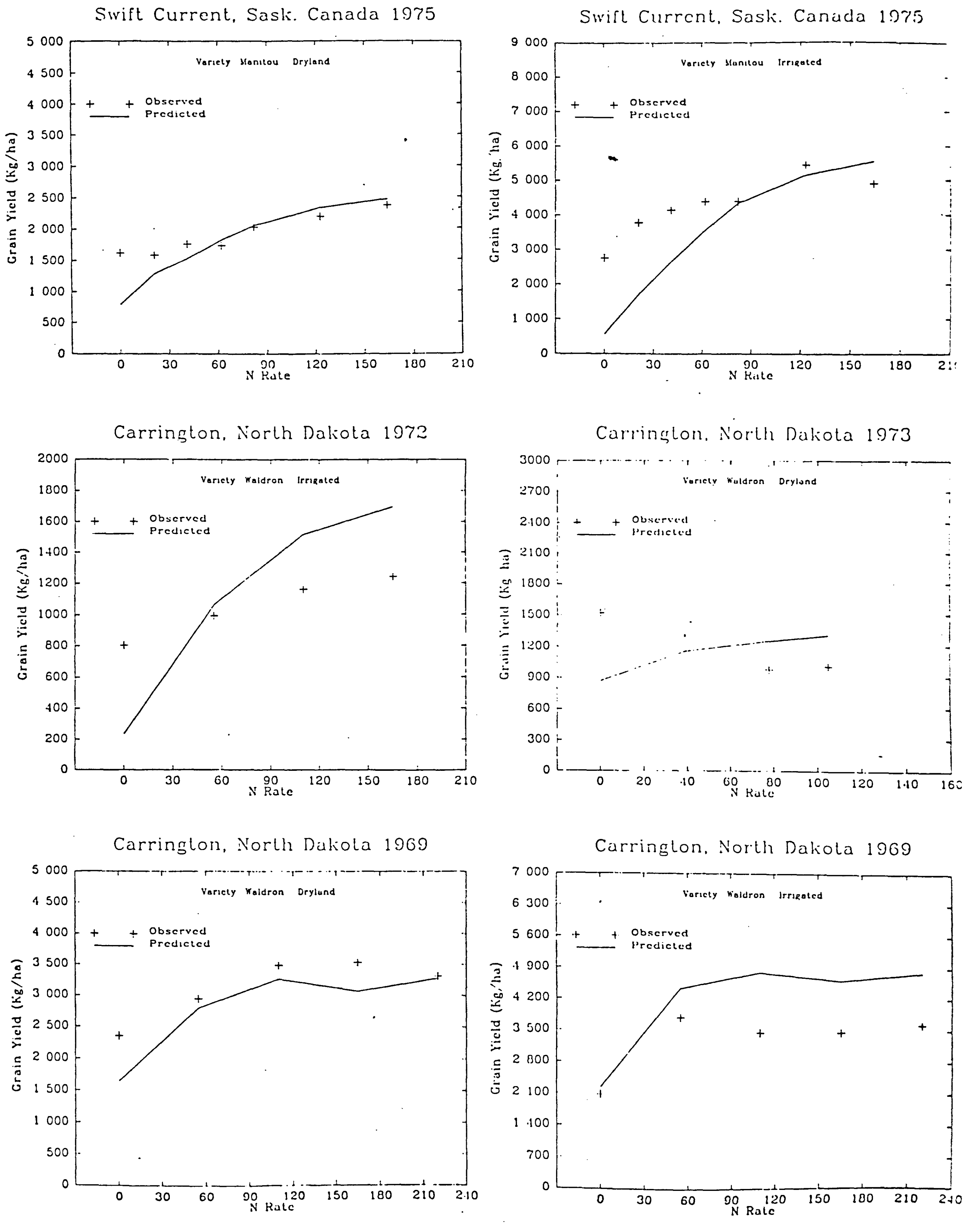

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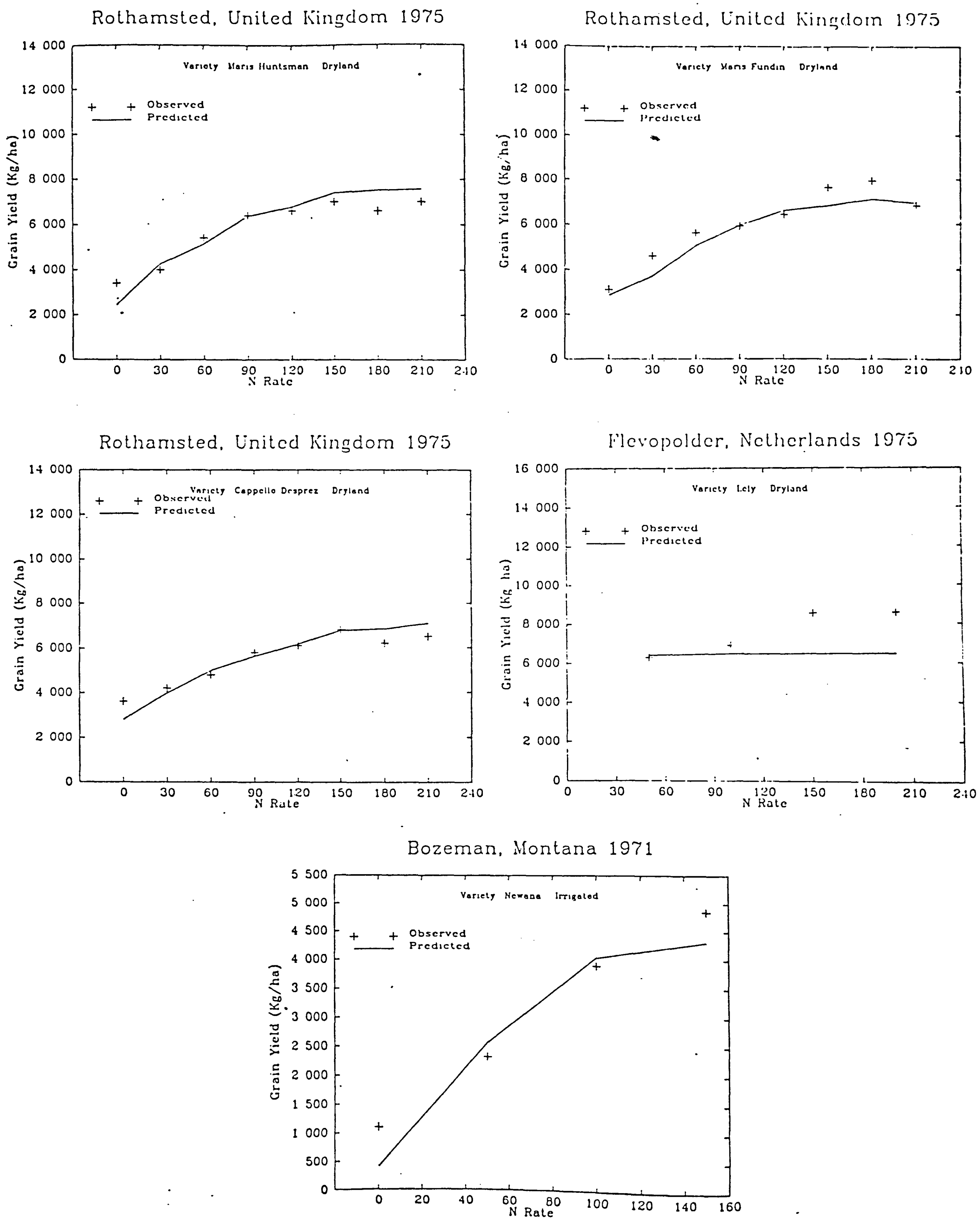

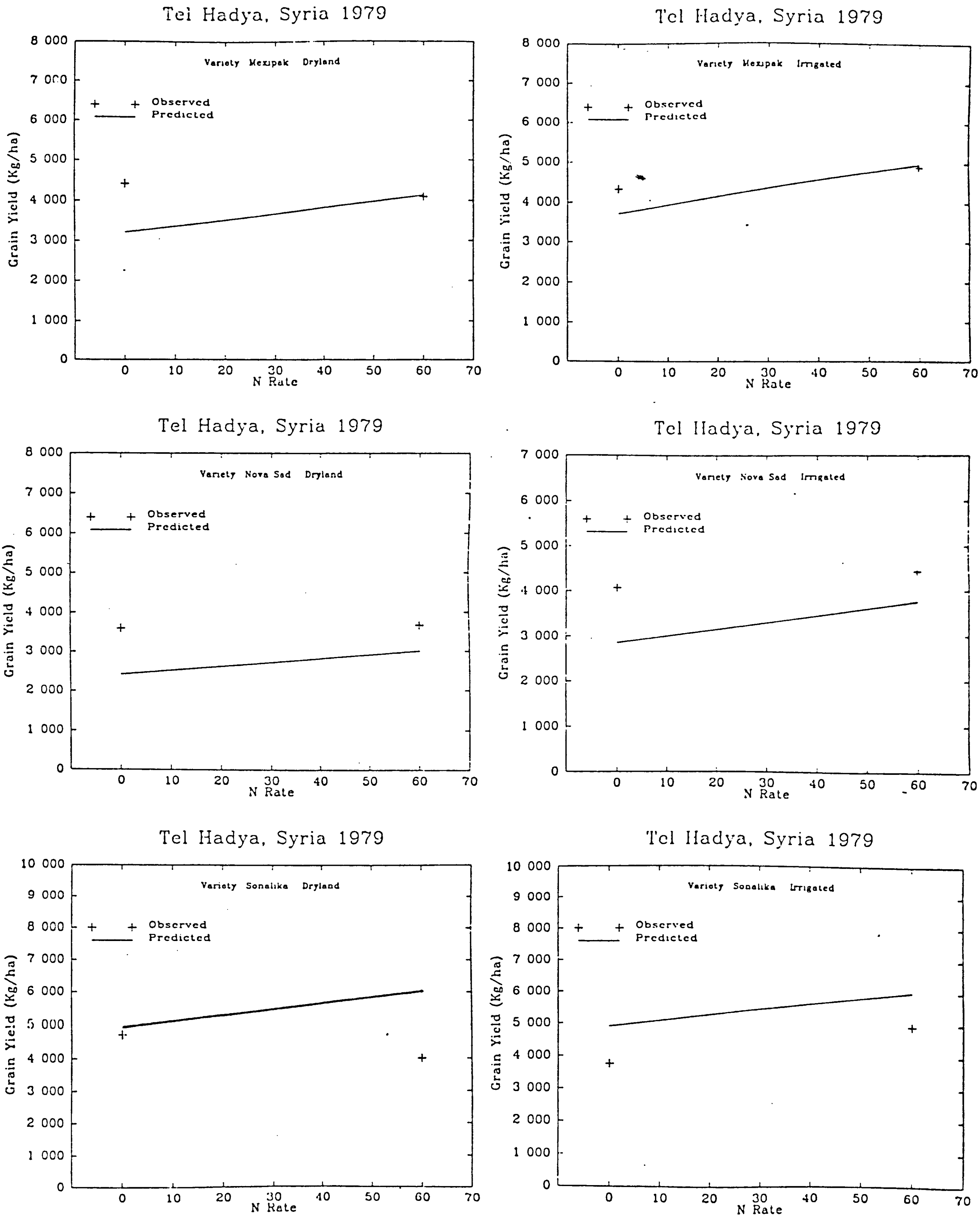

Figure 4.2. Continued.

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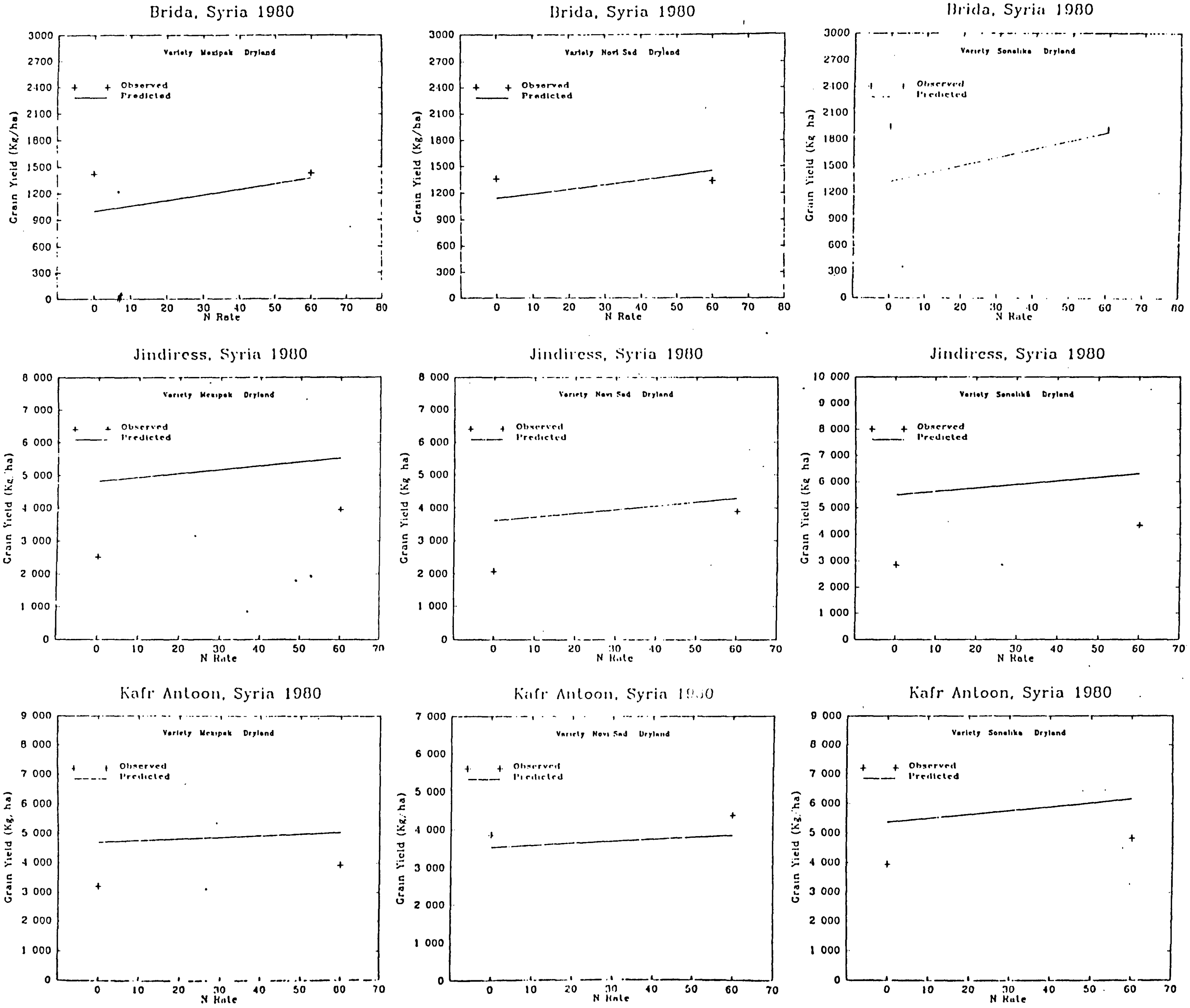
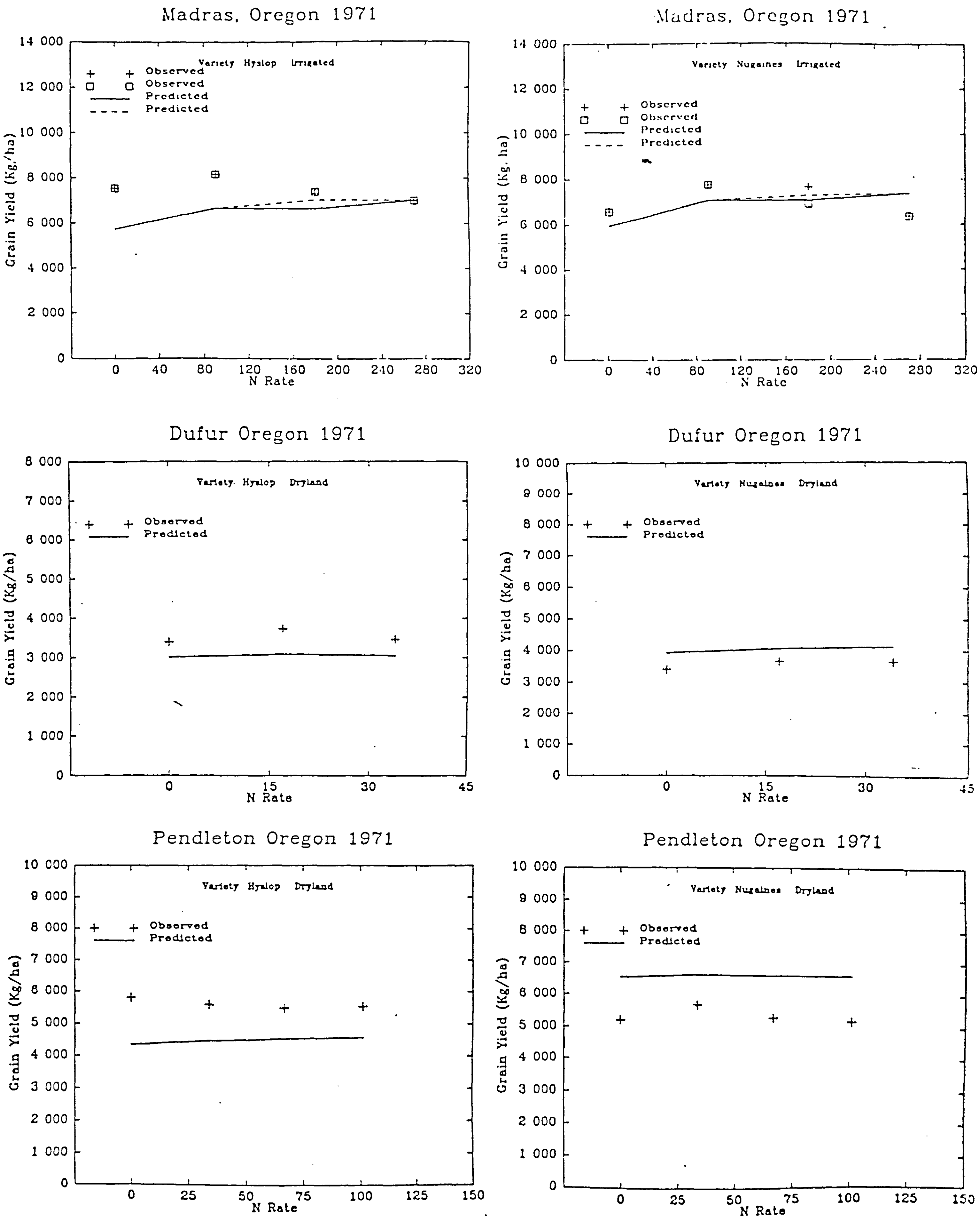
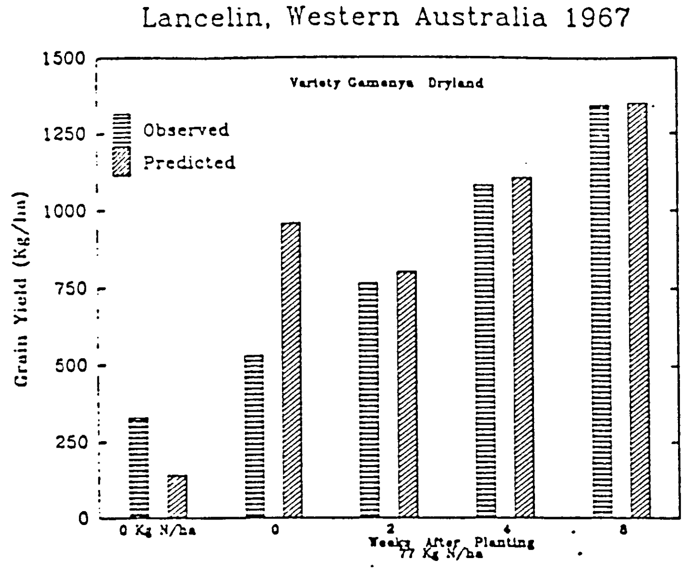
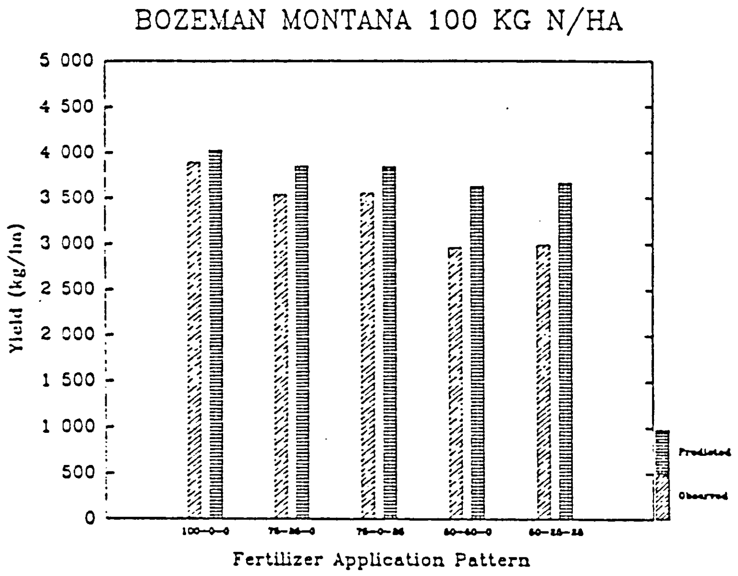


Figure 4.2. Continued.







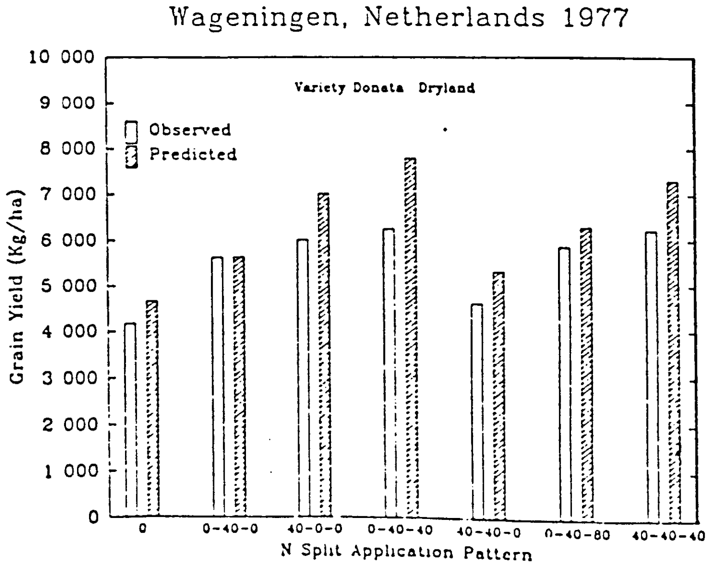


Figure 4.3. Comparison of Predicted and Observed Grain Yield Response to Differing Fertilizer Split Application Patterns.

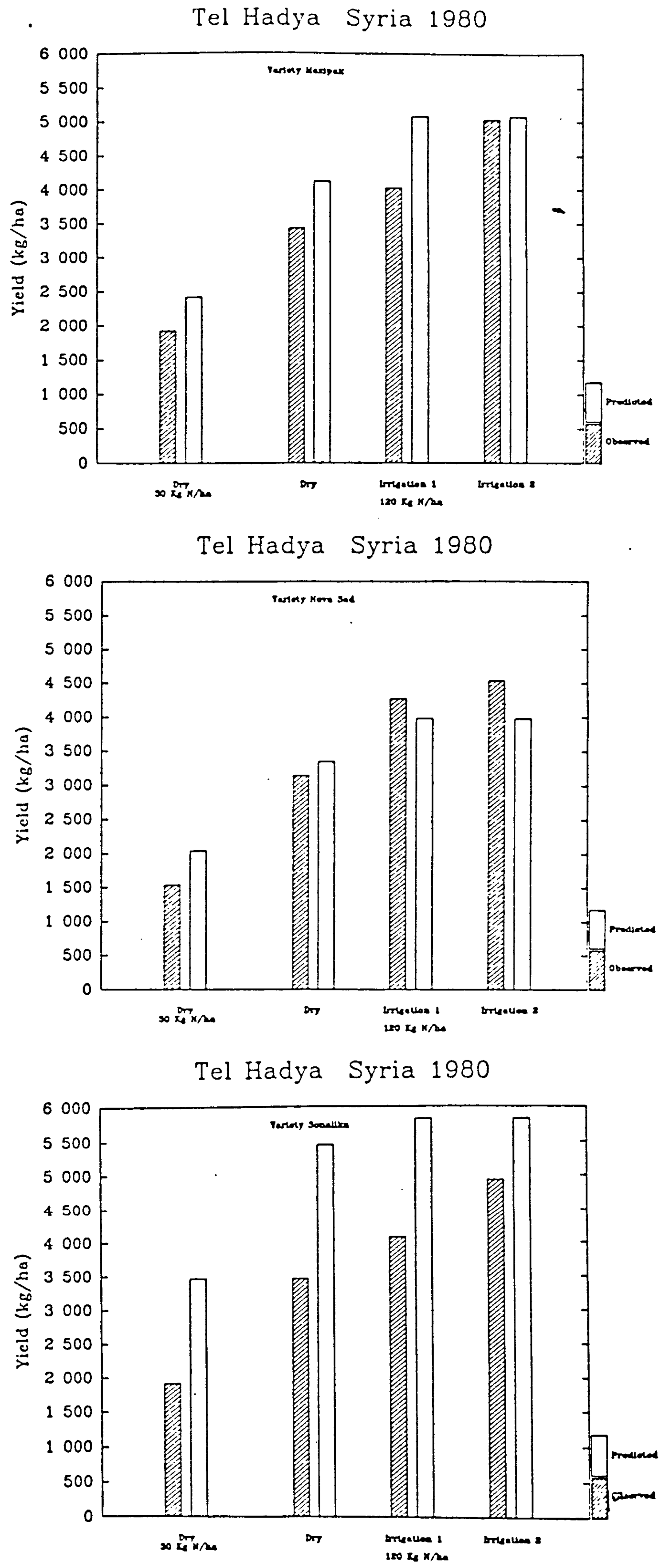


Figure 4.4. Comparison of Predicted and Observed Grain Yields at Differing Fertilizer Rates for Three Varieties With Different Irrigation Strategies.

in yield which was described by the model. Given the magnitude of the error for the Hutchinson data set compared to the other data sets from the same region, it is pertinent to question some of the input data and unusual phenomena associated with the experiment. Upon consultation with the authors involved (Wagger, personal communication) some suspicions about possible water runon due to the location of the experiment were raised but these could not be confirmed.

Marked responses to N in both years at Garden City, Kansas were not apparent in any of the irrigation treatments. The simulations reasonably approximated the observations across the range of treatments.

Predicted N responses for the Syrian data sets were, in general, very good. Yields for some of the varieties were overestimated at Jindiress and Kafr Antoon, but the simulations were consistent with the remarks noted above (see 4.2). Yields for the longer duration variety Novi Sad were overestimated at Tel Hadya 1979 and small underestimates of yield occurred for the zero N treatments at Brida.

Responses to N applied either at planting or in split applications were not apparent at Madras, Oregon or for single applications at Dufur. Simulations for each of these treatments were very close to the observations. The model underestimated yields for the variety Hyslop at Pendleton but overestimated yields across the range of N rates for the variety Nugaines.

The model underestimated the grain yield at low N rates in the Swift Current 1975 experiment but simulations for the remainder of the response curve were excellent. Excellent yield simulations were also recorded for the Rothamsted data sets.

The sensitivity of the model to differences in fertilizer application pattern (timing) are well illustrated by the data sets from Lancelin, Wageningen, and Bozeman (Figure 4.3).

The predicted and observed grain protein response to N application is plotted in Figure 4.5. Grain protein concentration, in general, was well simulated across the range of N rates except for the cases noted in 4.3.3. These exceptions rendered the simulation of grain protein to be unacceptable statistically when all data sets were combined. Given the constraints noted above in model development and the proximity of the majority of the simulations depicted in Figure 4.3, there is insufficient evidence to reject the model for the applications for which it was designed.

There was a general tendency for the model to overestimate total N uptake as noted in 4.3.3. There was no consistent pattern of overestimation or underestimation across the range of N rates employed in the various studies. Despite the problems indicated above in individual data sets the model captures most of the observed effects on N uptake for most of the data sets. Some further study is required to elucidate the problems with the North Dakota and Syrian data sets.

4.5. Seasonal Patterns of Biomass and N Uptake Accumulation

Across the range of data sets studied there was a consistent trend of predicted biomass being slightly out of phase with observed biomass (Figure 4.6). The model tended to predict higher biomass accumulations earlier in the season than the observations would indicate. While there was a noticeable trend the errors were, in general, not large and were consistent with those observed for the

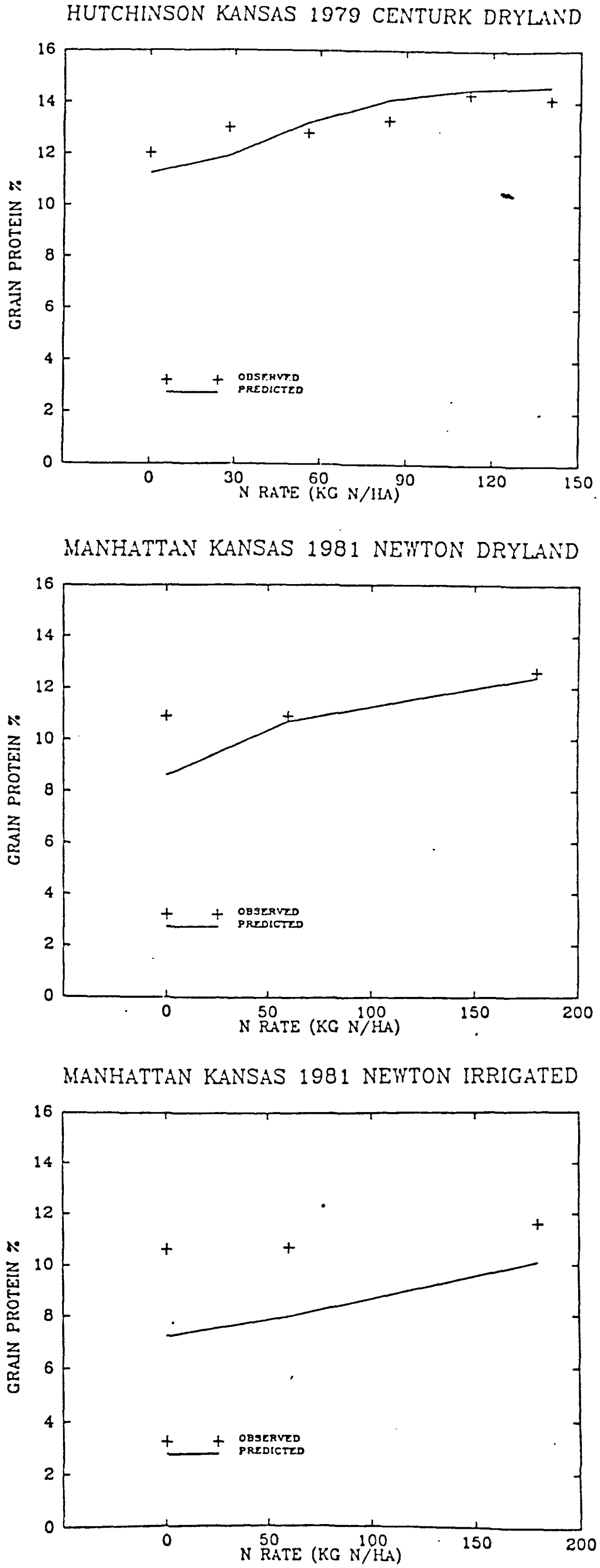
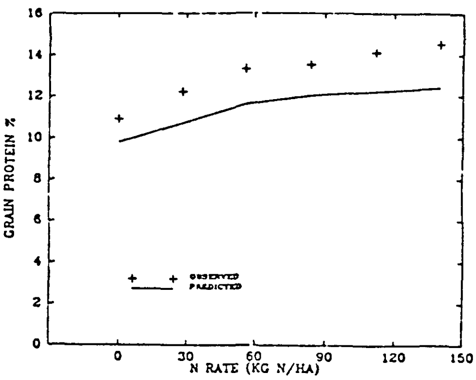


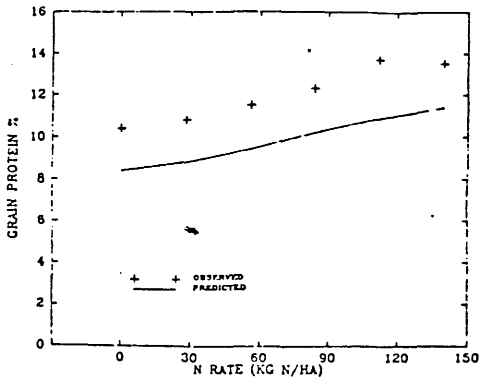
Figure 4.5. Comparison of Predicted and Observed Grain Protein Response to Applied N in Individual Data Sets.

Figure 4.5. Continued.

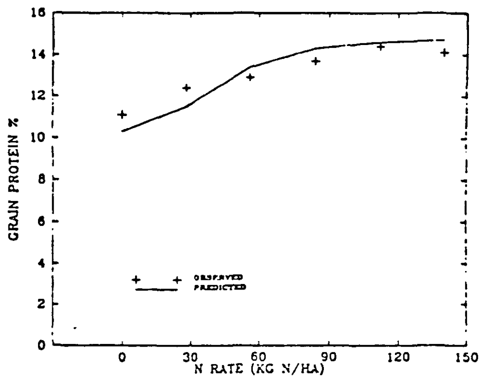
GARDEN CITY KANSAS 1980 NEWTON IRRIGATION 1



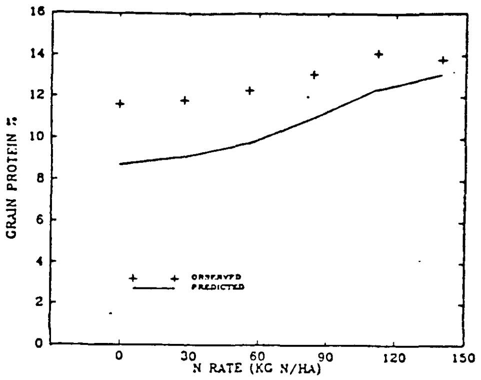
GARDEN CITY KANSAS 1980 NEWTON IRRIGATION 2



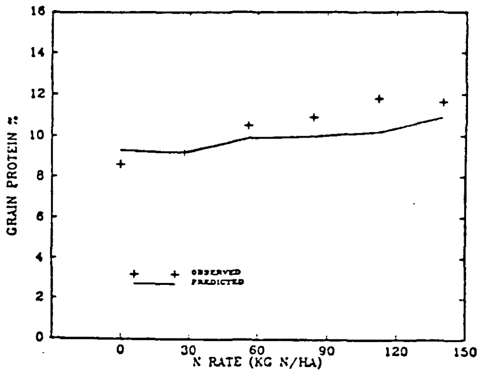
GARDEN CITY KANSAS 1980 NEWTON IRRIGATION 3



GARDEN CITY KANSAS 1980 NEWTON IRRIGATION 4



GARDEN CITY KANSAS 1981 NEWTON IRRIGATION 1



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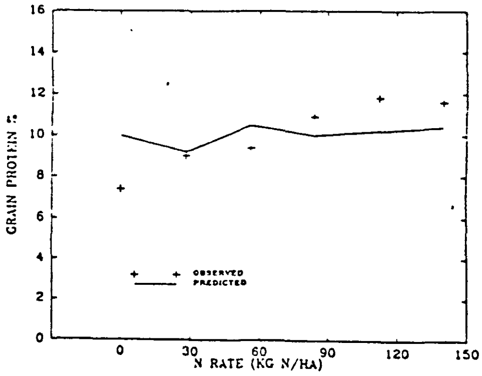

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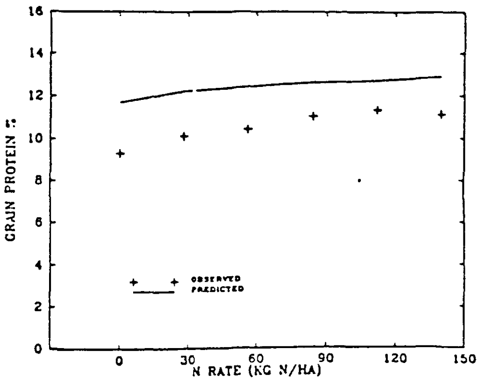

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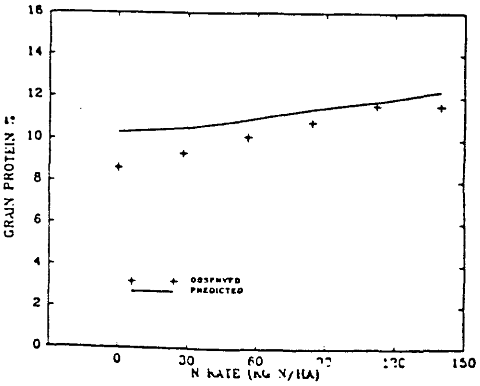
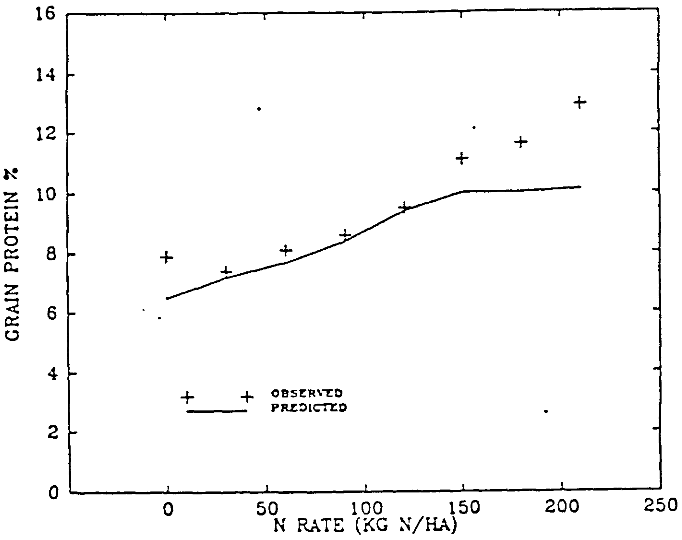
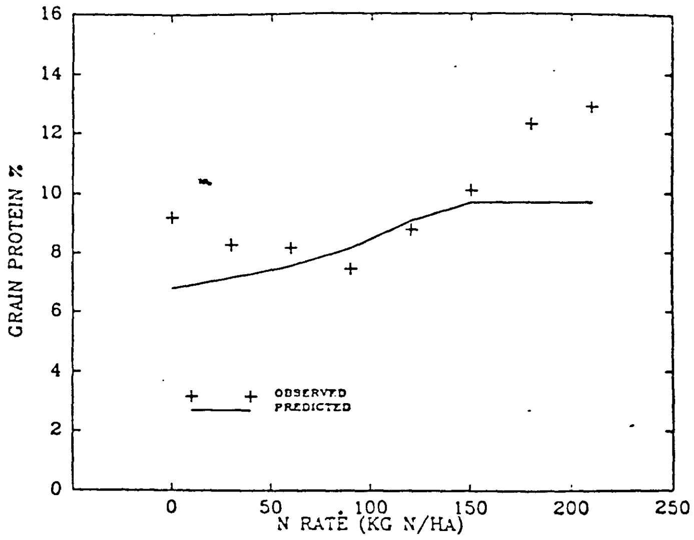


Figure 4.5. Continued.

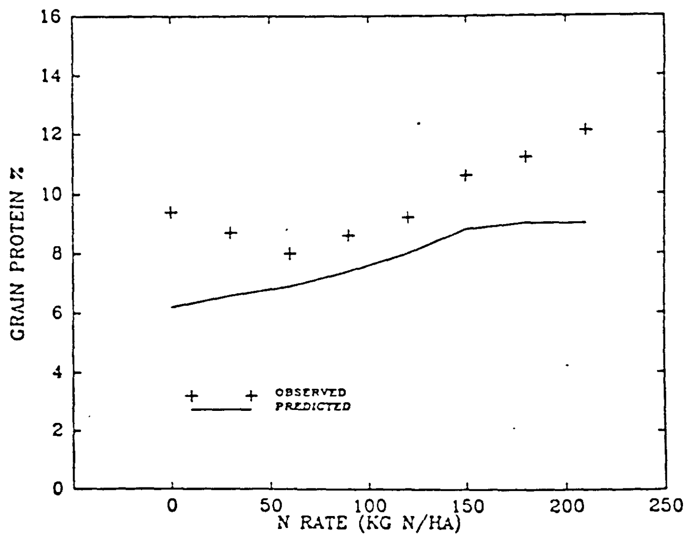
ROTHAMSTED ENGLAND 1975 MARIS HUNTSMAN DRYLAND



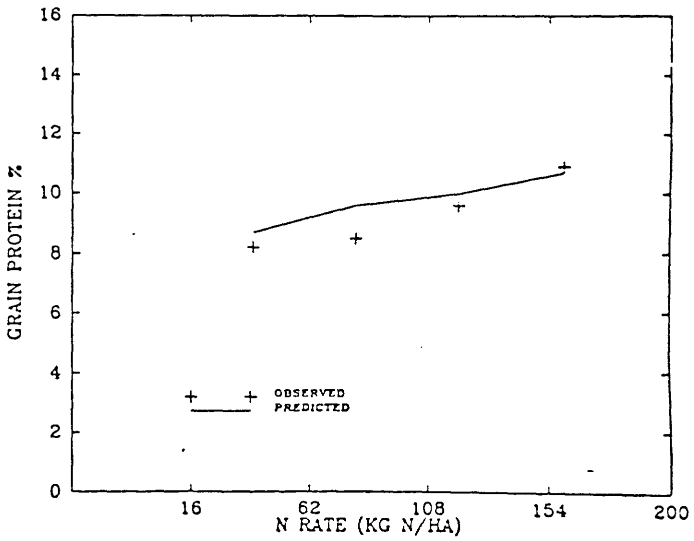
ROTHAMSTED ENGLAND 1975 MARIS FUNDIN DRYLAND



ROTHAMSTED ENGLAND 1975 CAPELLE DESPREZ DRYLAND



WAGENINGEN NETHERLANDS 1977 SPLIT APPLICATIONS DONATA



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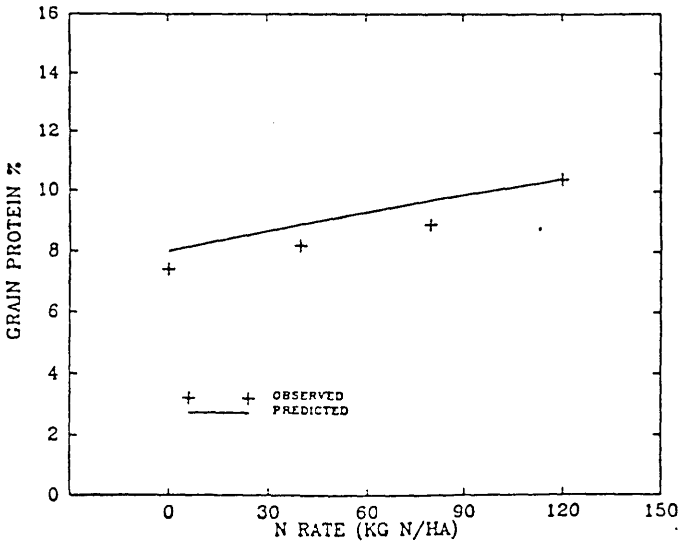
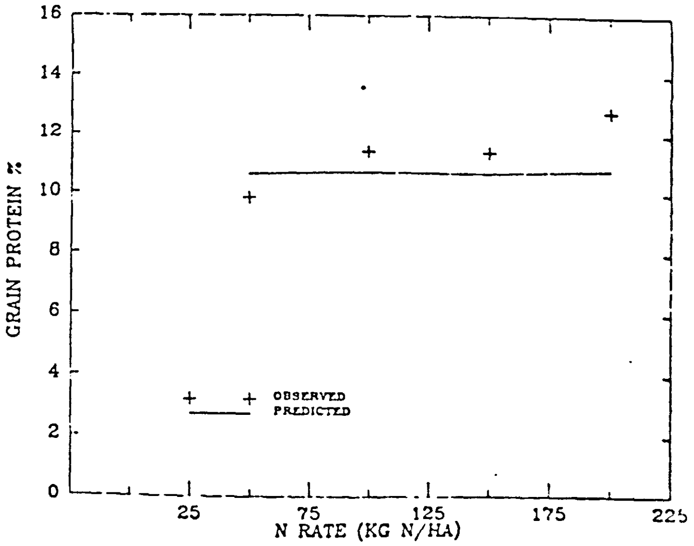


FLEVOPOLDER NETHERLANDS 1975 LELY



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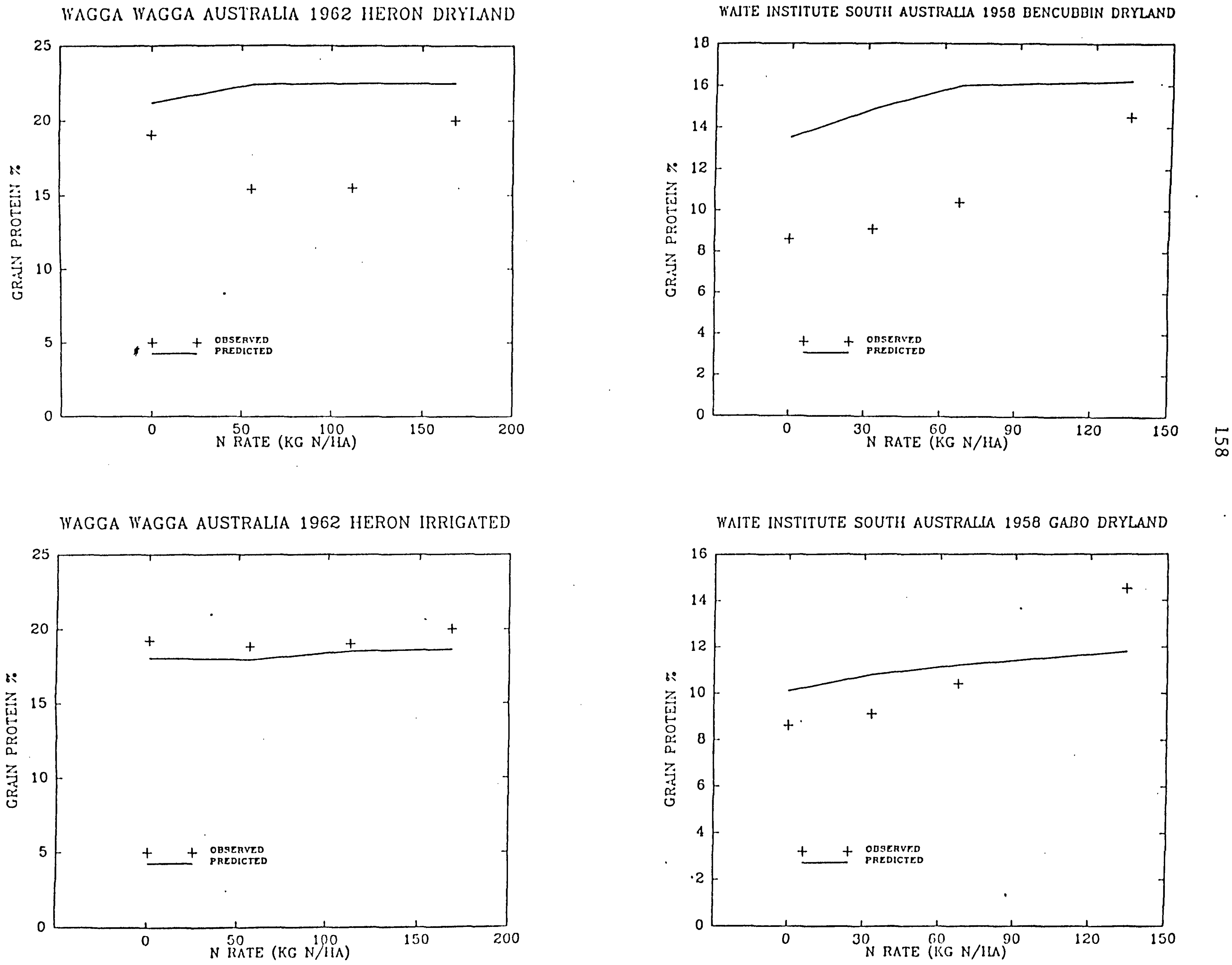


WAGGA WAGGA AUSTRALIA 1962 HERON DRYLAND

WAITE INSTITUTE SOUTH AUSTRALIA 1958 BENCUBBIN DRYLAND

WAGGA WAGGA AUSTRALIA 1962 HERON IRRIGATED

WAITE INSTITUTE SOUTH AUSTRALIA 1958 GABO DRYLAND

Figure 4.5. Continued.

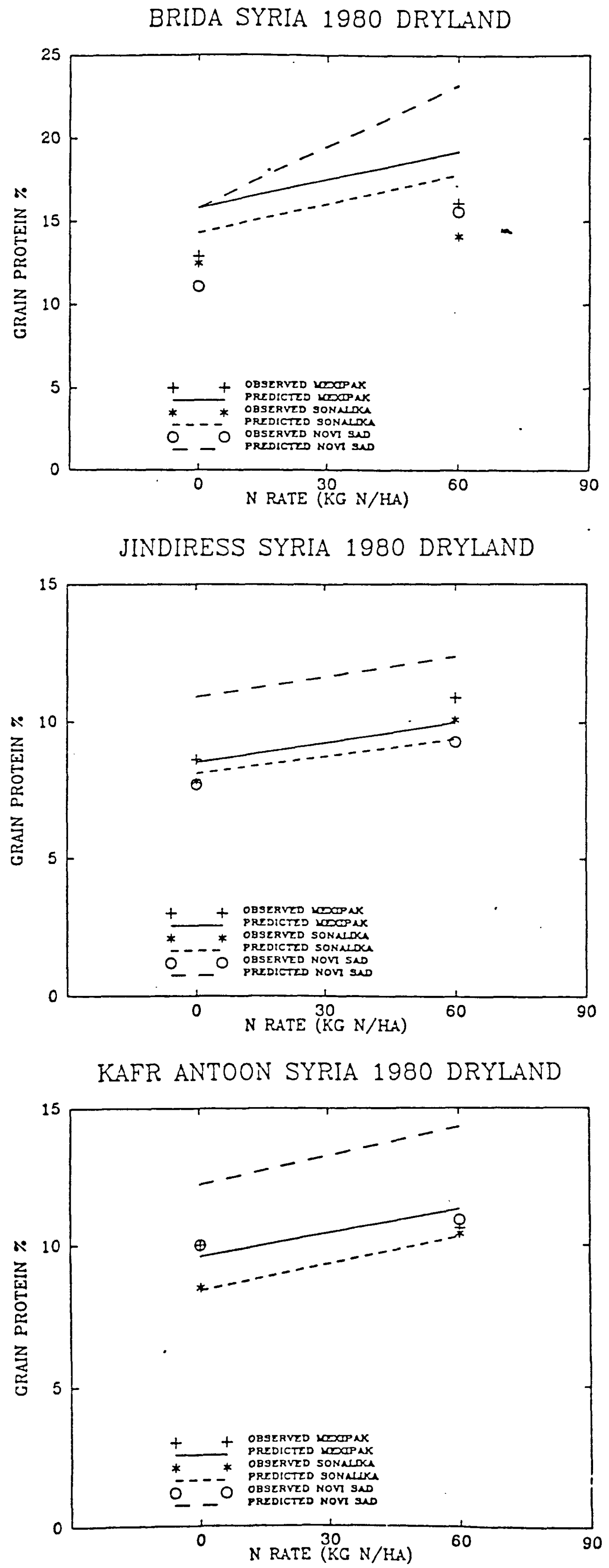
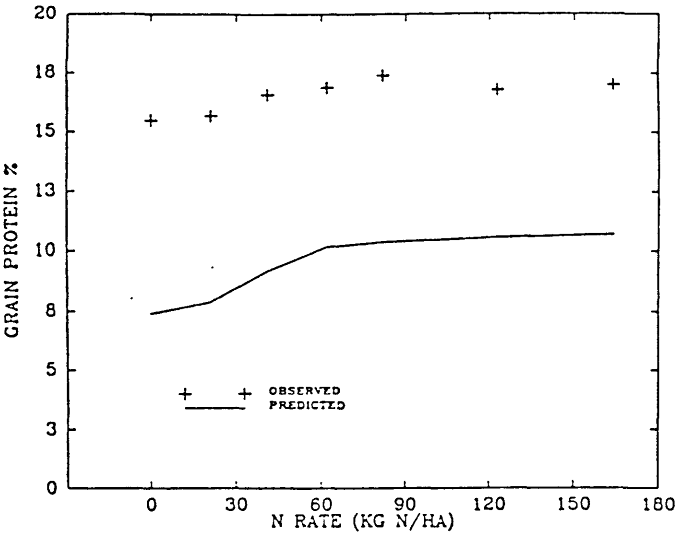
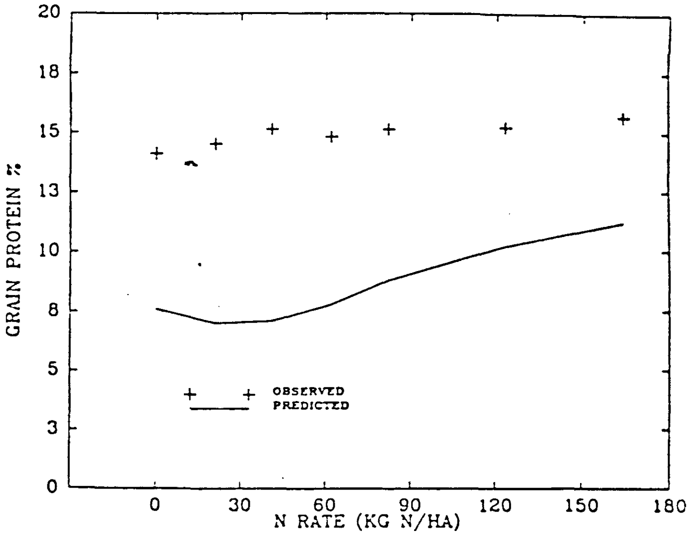


Figure 4.5. Continued.

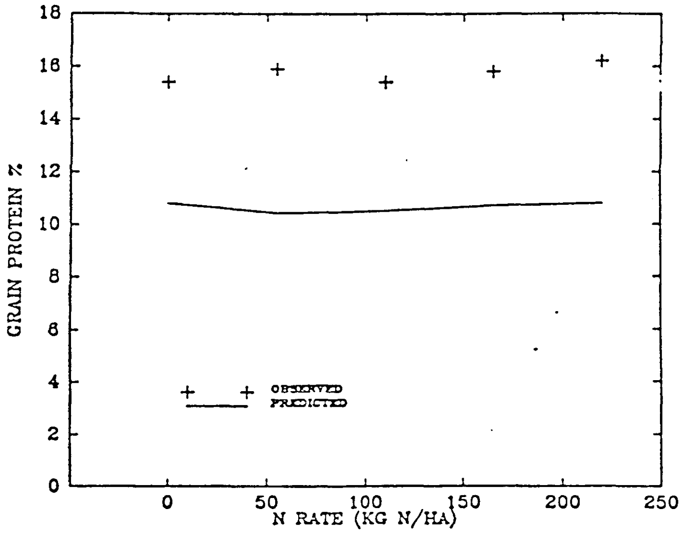
SWIFT CURRENT SASKATCHEWAN 1975 MANITOU DRYLAND



SWIFT CURRENT SASKATCHEWAN 1975 MANITOU IRRIGATED



CARRINGTON NORTH DAKOTA 1969 WALDRON DRYLAND



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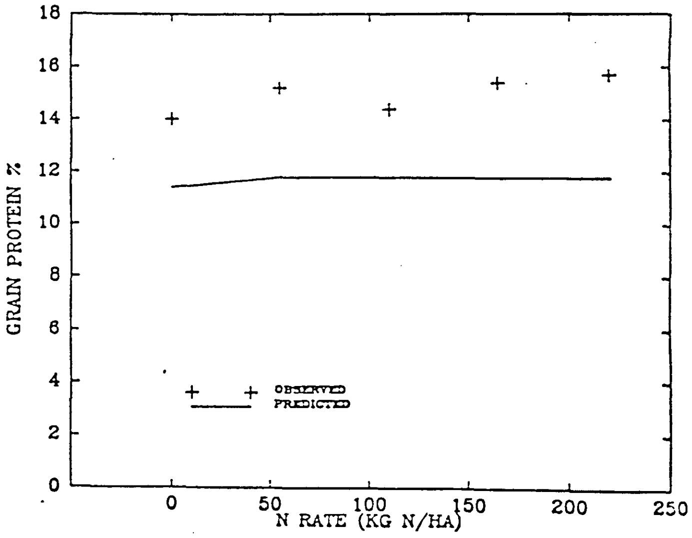

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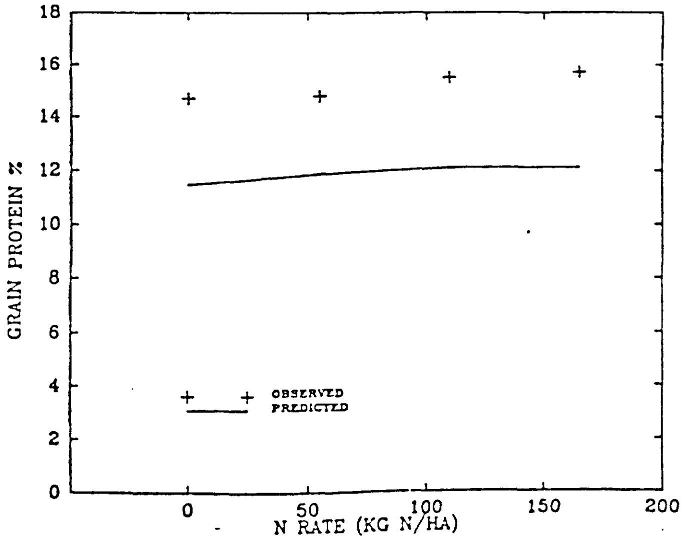

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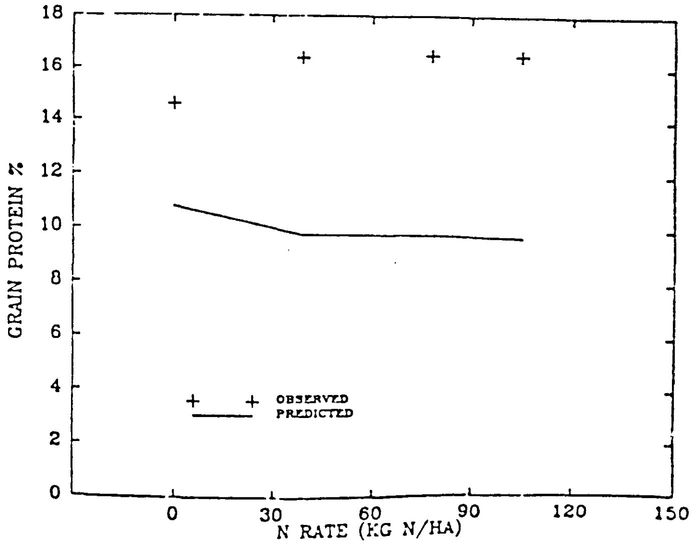

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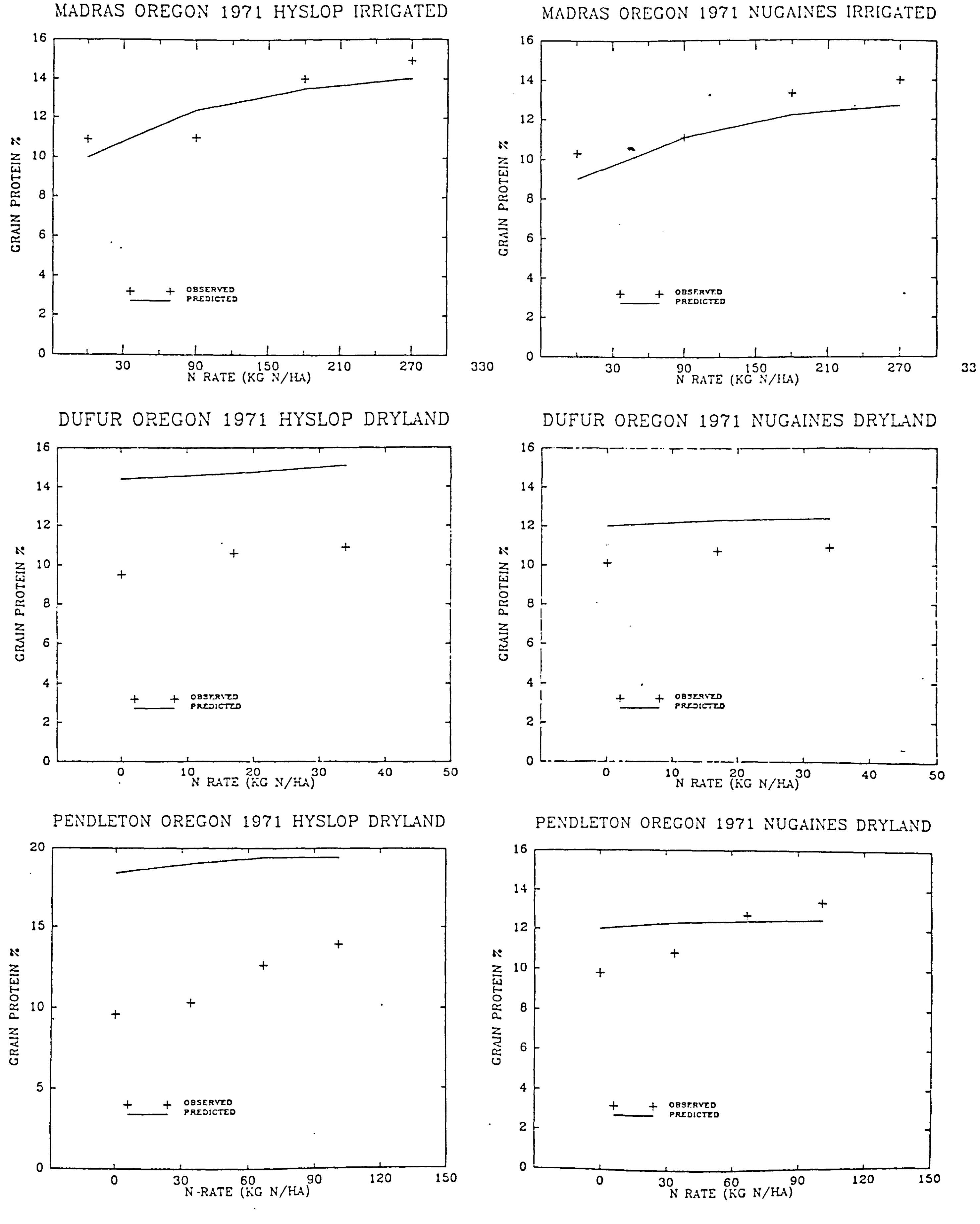


MADRAS OREGON 1971 HYSLOP IRRIGATED

MADRAS OREGON 1971 NUGAINES IRRIGATED

DUFUR OREGON 1971 HYSLOP DRYLAND

DUFUR OREGON 1971 NUGAINES DRYLAND

PENDLETON OREGON 1971 HYSLOP DRYLAND

PENDLETON OREGON 1971 NUGAINES DRYLAND

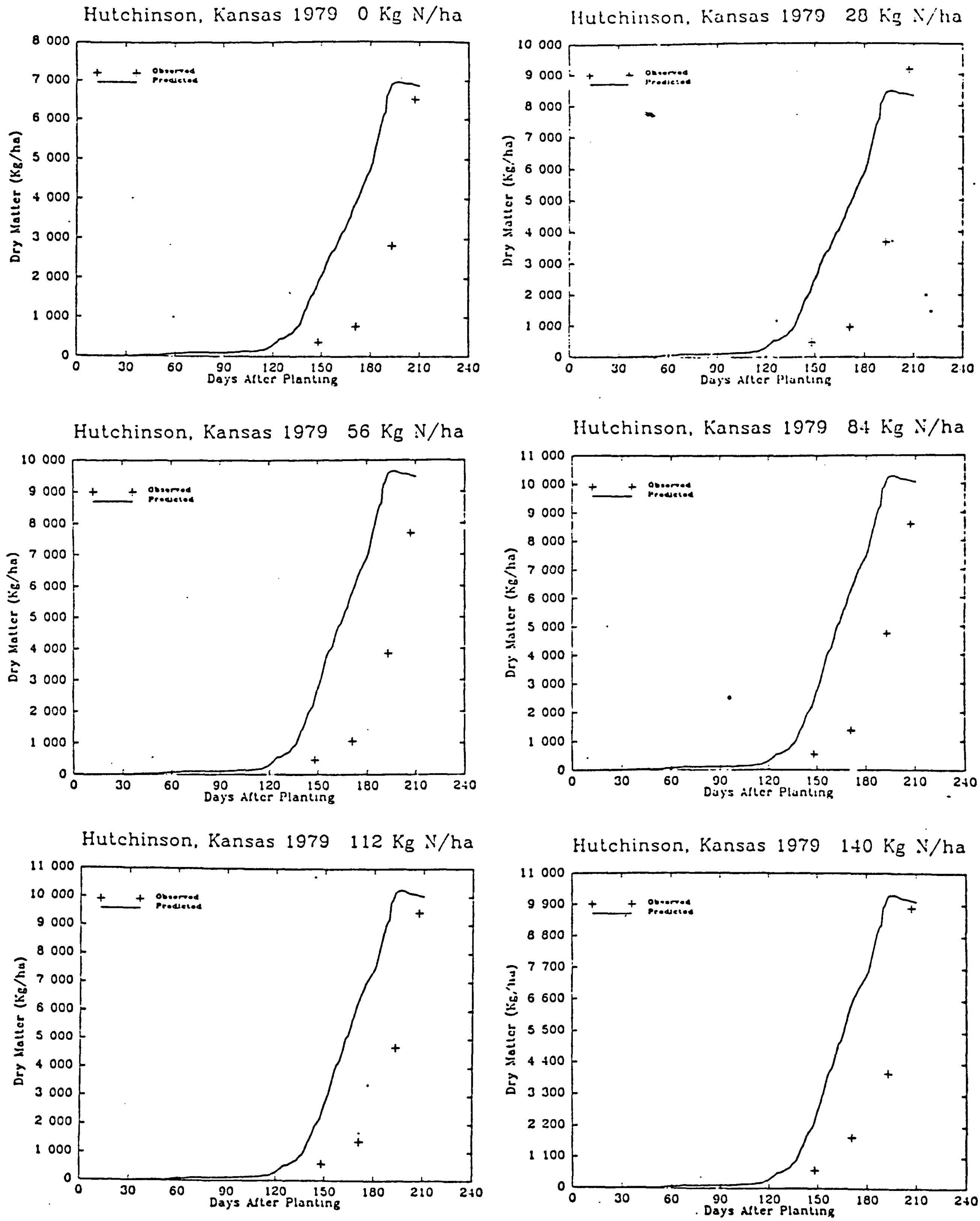
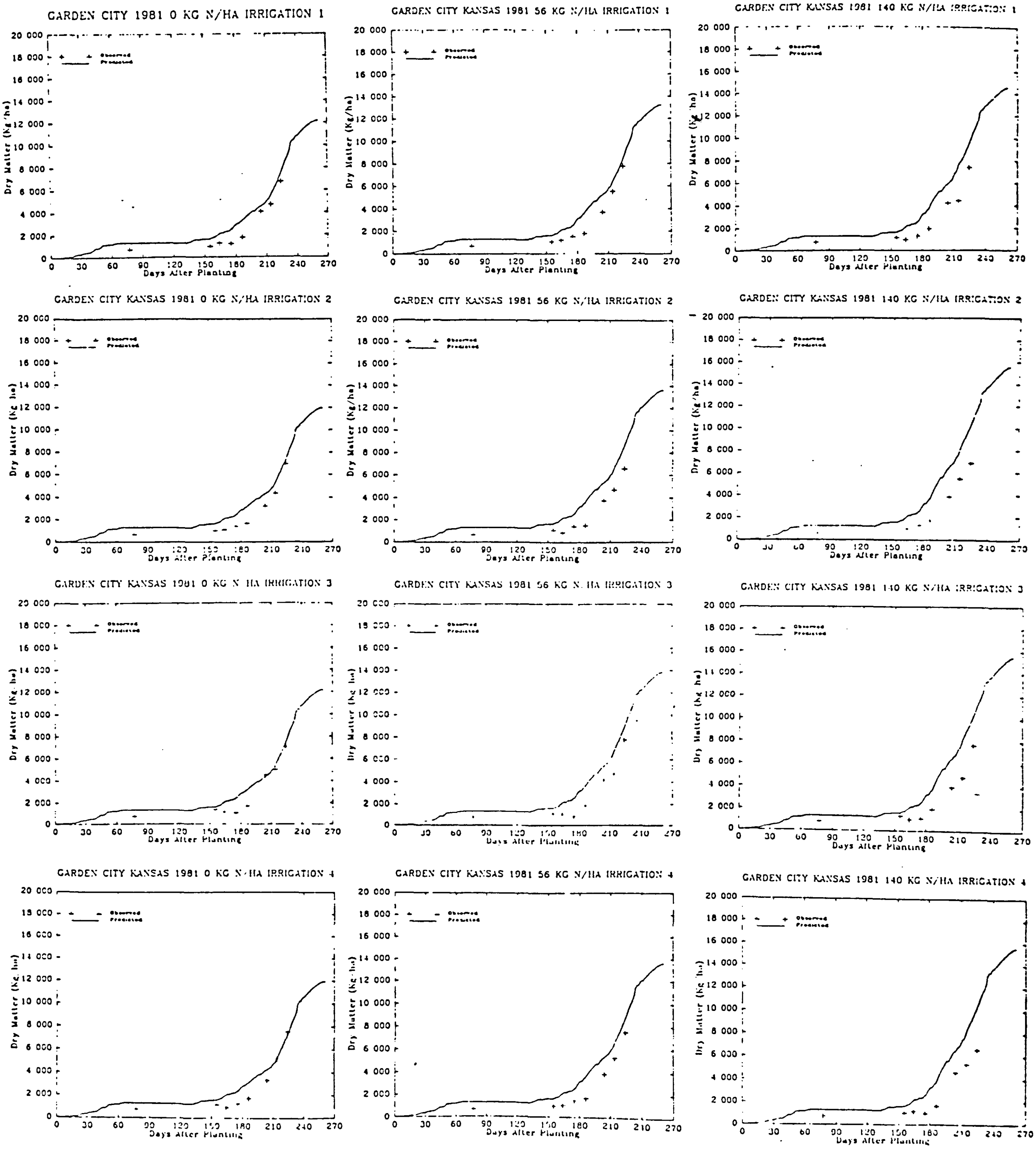


Figure 4.6. Comparison of Predicted and Observed Seasonal Dry Matter Production for Individual Data Sets.

Figure 4.6. Continued.



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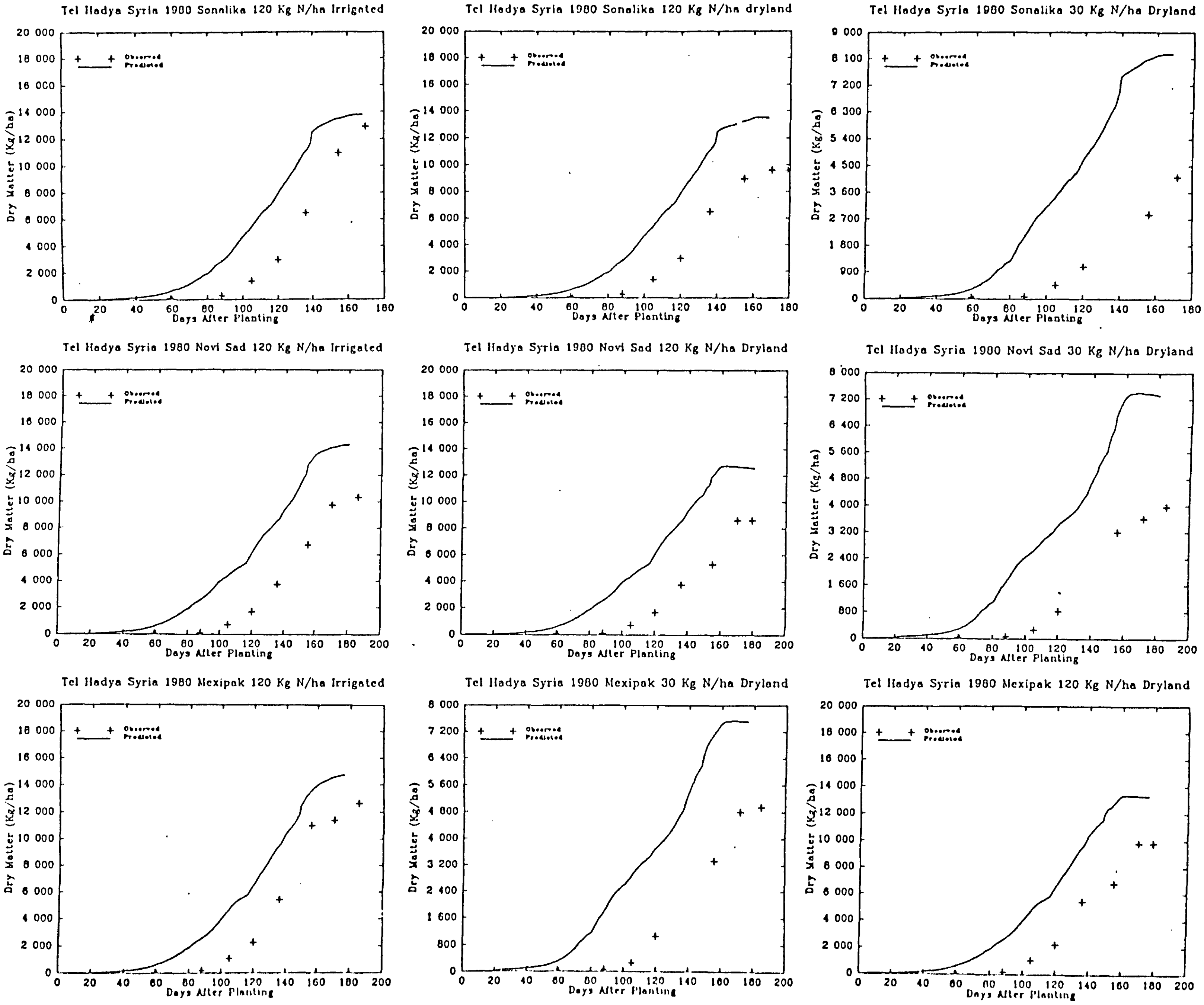
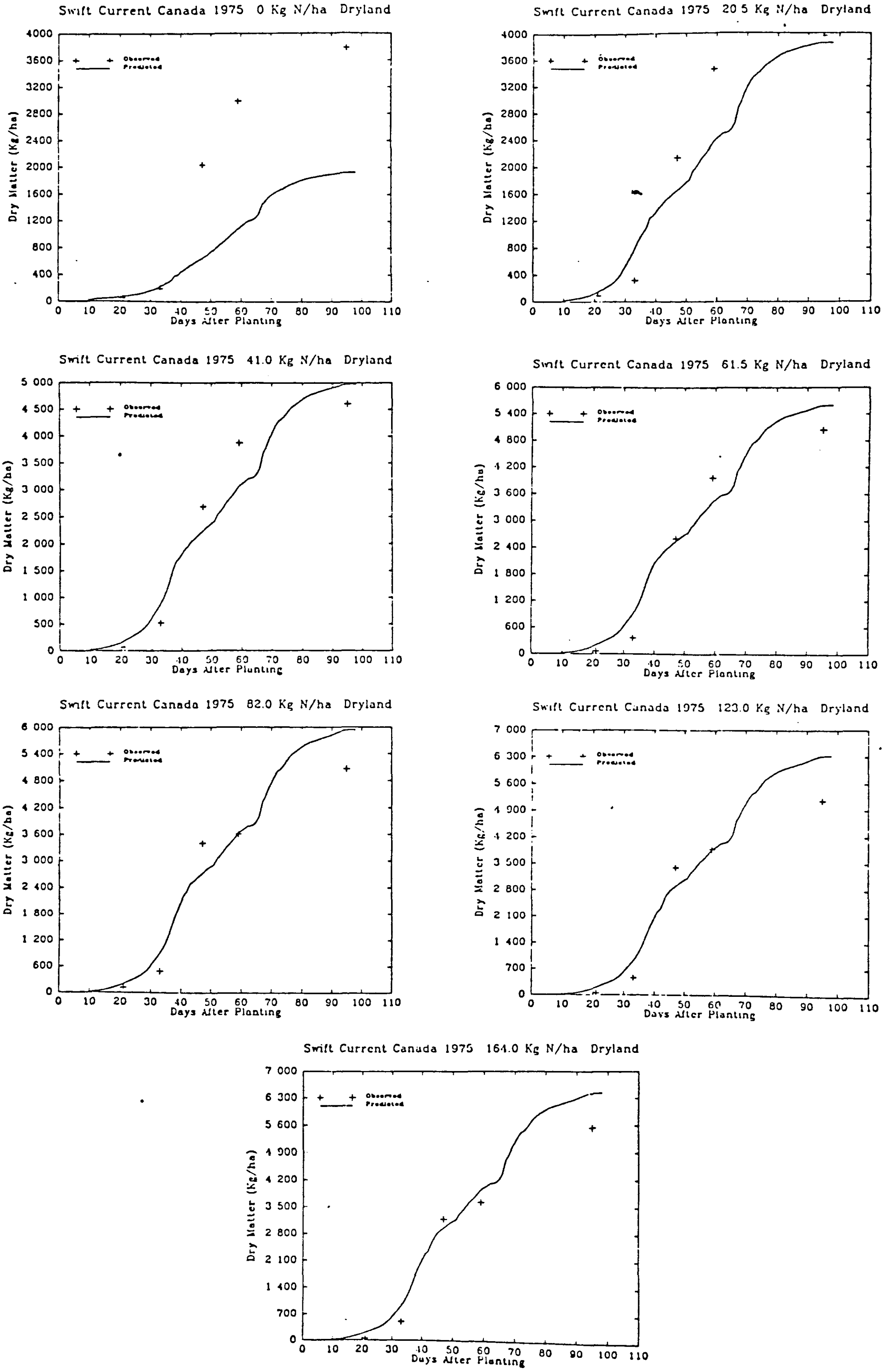


Figure 4.6. Continued.



Swift Current Canada 1975 0 Kg N/ha Dryland

Swift Current Canada 1975 20.5 Kg N/ha Dryland

Swift Current Canada 1975 41.0 Kg N/ha Dryland

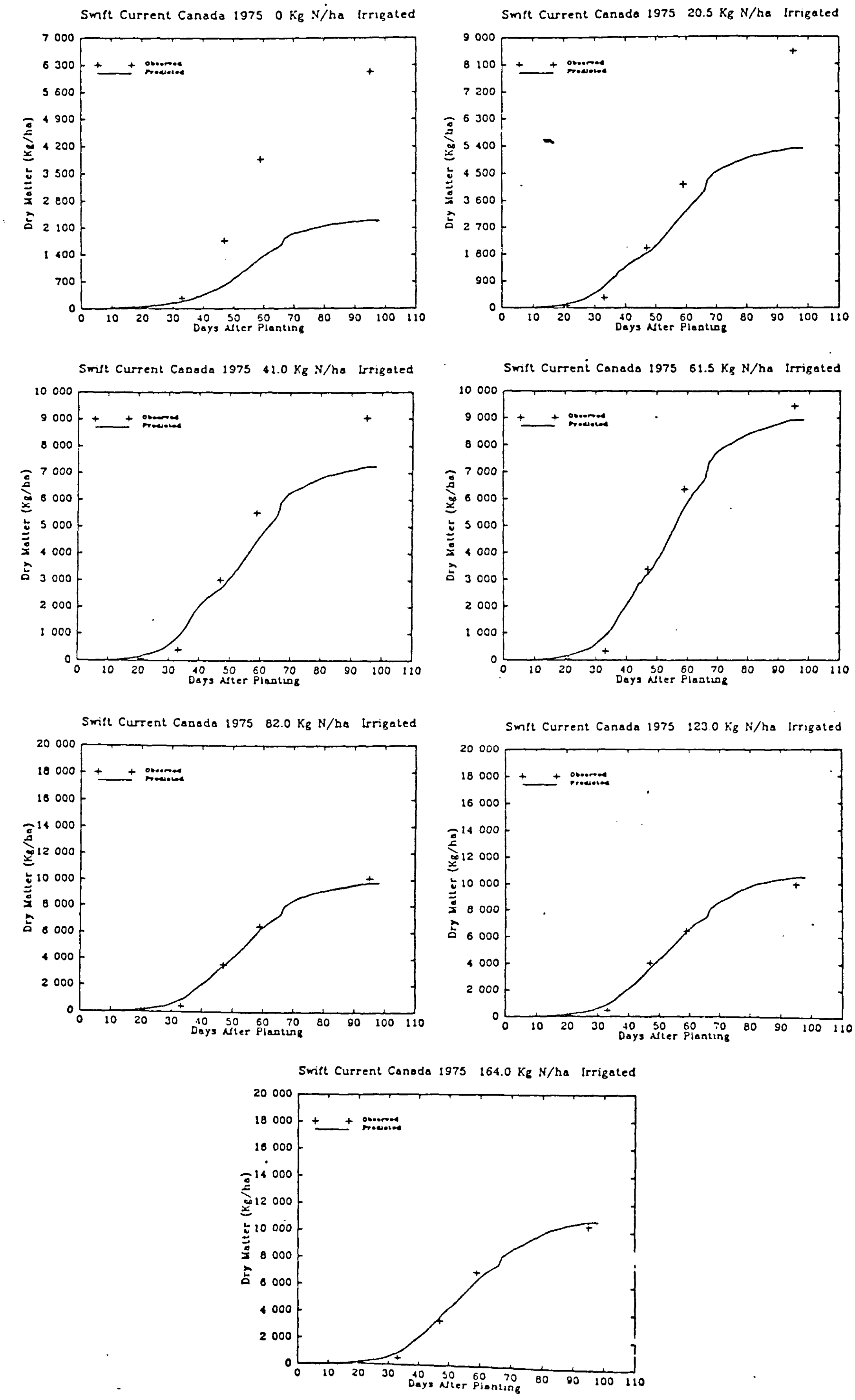
Swift Current Canada 1975 61.5 Kg N/ha Dryland

Swift Current Canada 1975 82.0 Kg N/ha Dryland

Swift Current Canada 1975 123.0 Kg N/ha Dryland

Swift Current Canada 1975 164.0 Kg N/ha Dryland

Figure 4.6. Continued.



non-nitrogen version of the model (Otter-Nacke et al., 1986). Errors were large, however, at the low N rates for the Swift Current data set and for some treatments in the Tel Hadya 1980 data set.

Not surprisingly, a similar pattern in seasonal N uptake (Figure 4.7) to that obtained for biomass was observed (i.e., some tendency for an early overestimation of N uptake). Seasonal patterns of N uptake were poorly simulated at the low N rates in the Swift Current data set but reasonably simulated in the Kansas data sets.

4.6. Seasonal Patterns of Nitrogen Balance

When attempting the validation of the soil nitrogen components of the model, it was originally intended to attempt a layer by layer comparison of each of predicted nitrate and ammonium concentrations with those observed. Analysis of the observed data in most instances firstly indicated very large standard errors, and other seeming anomalies were sometimes apparent. In some of the data sets mineral N concentrations were low after fertilizer addition and increased as the crop grew and withdrew N from the soil. While this may be indicative of turnover occurring within the soil systems, due to microbial activity or ammonium adsorption/desorption on clay surfaces, in some cases the anomalies in the individual layers were so gross as to discard many of them.

Validation of the nitrogen balance component of the model is attempted by examining predicted and observed seasonal changes in gains and losses of N from the soil/plant system as outlined in 4.1. In the three data sets selected for this analysis, net mineralization occurs during the season in most of the treatments in the Swift Current data set. This is particularly so in the irrigated treatments. In the Manhattan data set, small net losses occur in the dryland

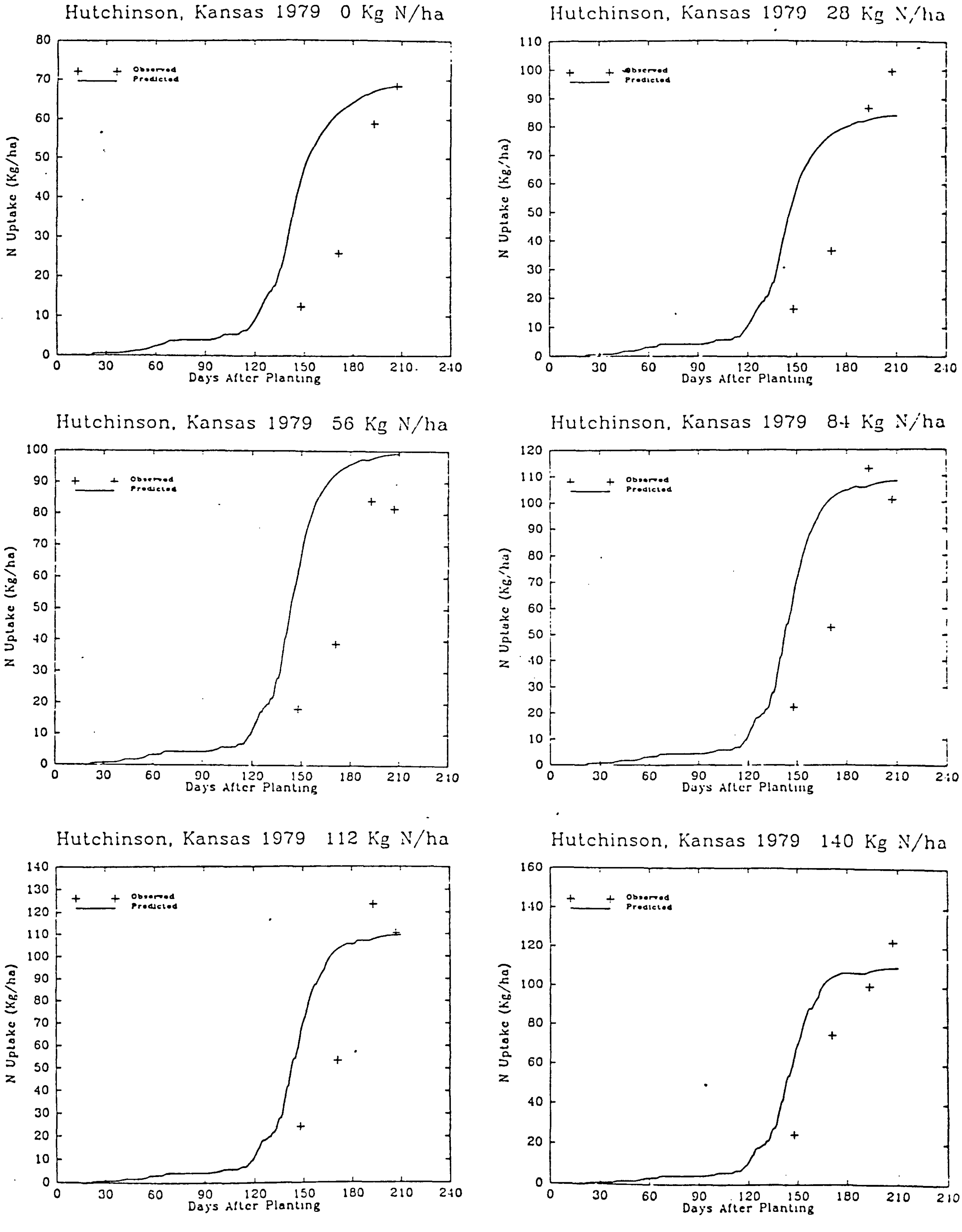


Figure 4.7. Comparison of Predicted and Observed Seasonal Pattern of N Uptake for Individual Data Sets.

Figure 4.7. Continued.

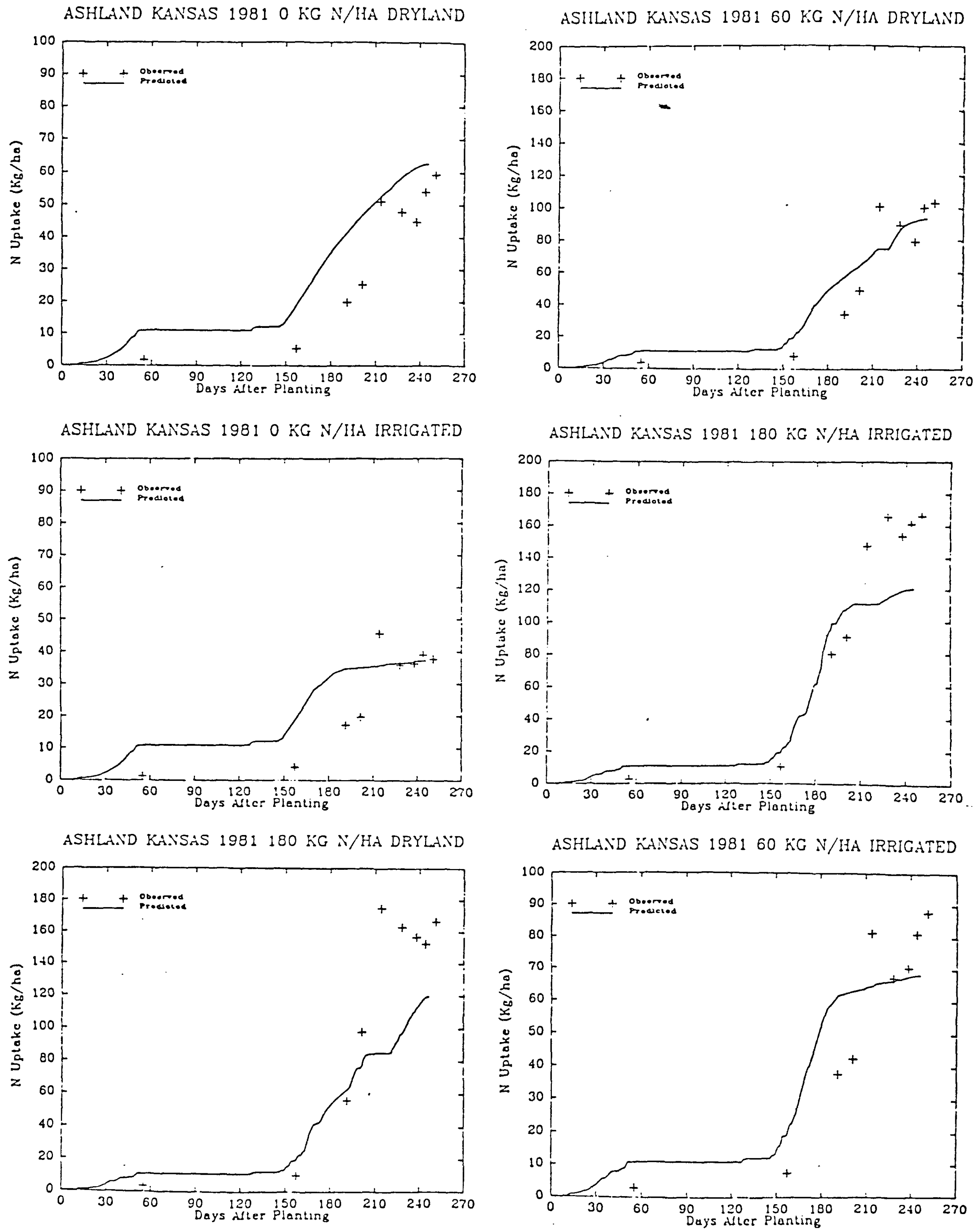
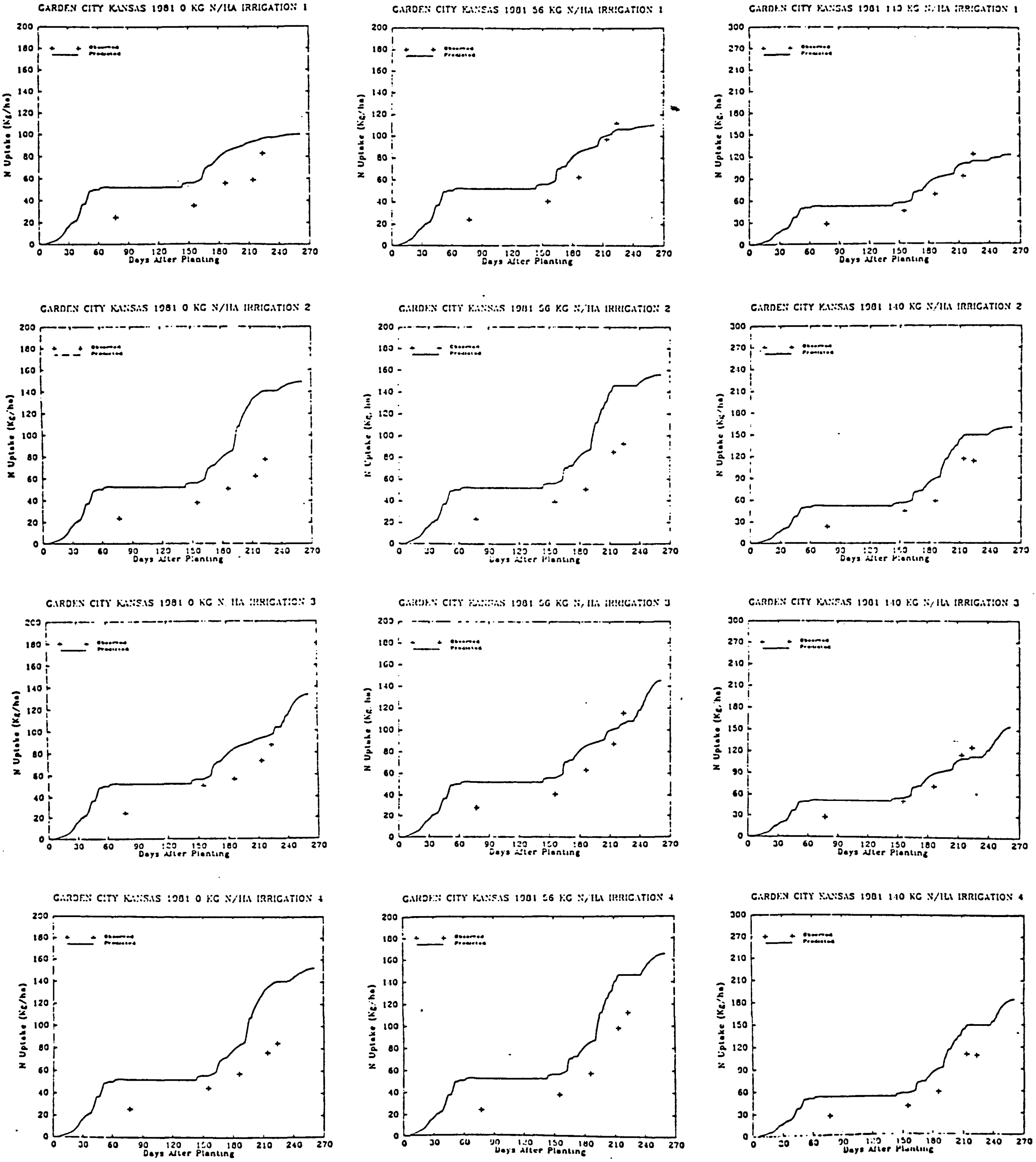


Figure 4.7. Continued.



treatments with larger losses (presumably through leaching) in the irrigated treatments. Data from ^{15}N-labelled crop residues in an experiment at the same site (Wagger, 1983) indicated that considerable net mineralization occurs during the season, but this is offset by N losses. In the Lancelin data set, heavy leaching losses occur from all treatments where the fertilizer was applied early. These data sets thus provide a full range of net gains and losses of N from the system. Overall, the model predicted "accountable N" reliably using the indicators tabulated in Table 4.1. Examination of Figure 4.8 indicates performance at Swift Current and Manhattan was better than at Lancelin. Errors in prediction at Lancelin may be due to an underestimation of the rate of leaching or to an underestimation of the rate of nitrification with more N being retained in the ammonium form and thus withheld from leaching. The seasonal patterns of N balance (Figure 4.9) further verify that the simulations of "accountable N" match observations closely. Some discrepancy in the predicted balance between soil and plant N, and between straw and grain occurs during the season, but in general this is not large.

4.7. Conclusions

CERES-Wheat-N is designed as a management-oriented model to be useful for a great diversity of applications in a great diversity of environments. To enable the model to be sufficiently general, and to be useful to such a wide audience, requires that the number of inputs used must be the minimum which could be reasonably attained or estimated from standard agricultural experimental practice. Given these constraints, the model proved able to simulate crop growth and response to fertilizer reasonably reliably. The rigorous statistical analysis did indicate some problems have yet to be resolved with the prediction of N uptake and grain protein concentration in some data sets. Some tendency to overpredict biomass and N uptake early in the season was noted. Further testing and refinement of this area of the model may bear fruit. Further data sets are required for rigorously testing the soil N components of the model.

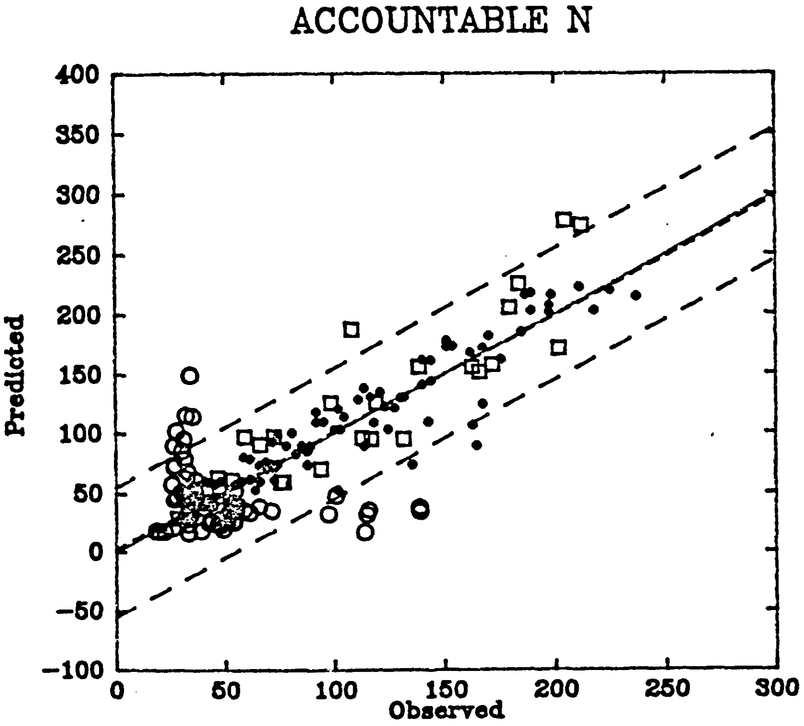


Figure 4.8. Comparison of Observed and Predicted Values of "Accountable N."

□ Manhattan Experiment.
o Lancelin Experiment.
• Swift Current Experiment.

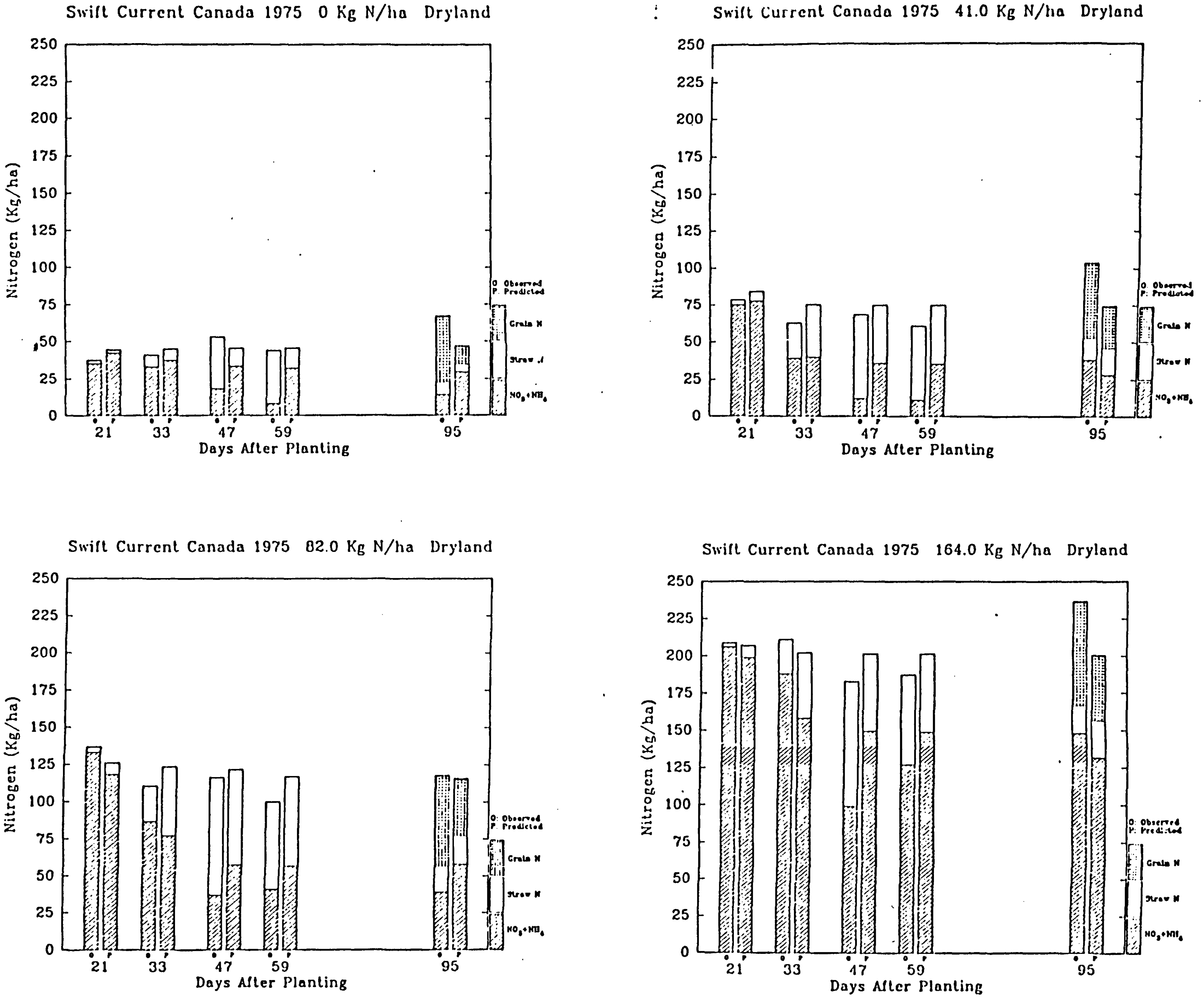


Figure 4.9. Comparison of Predicted and Observed Patterns in Seasonal N Balance for Individual Data Sets.

Figure 4.9. Continued.

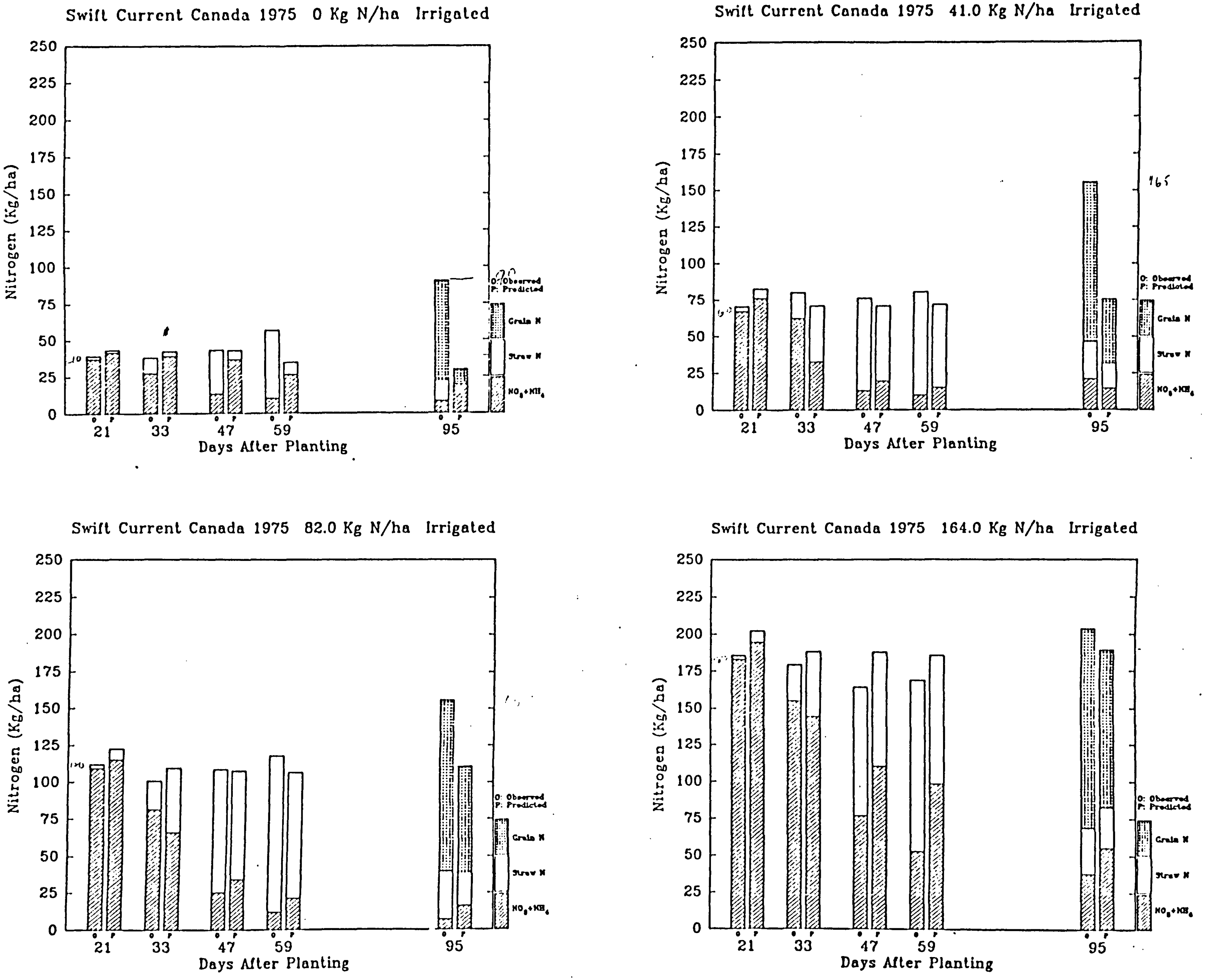
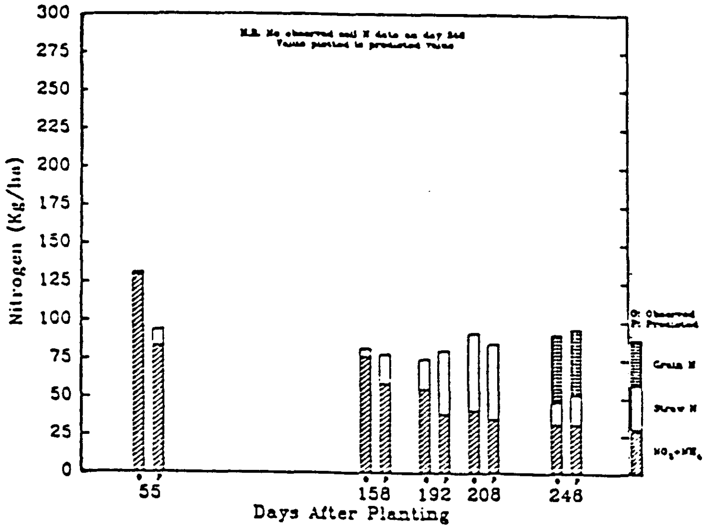
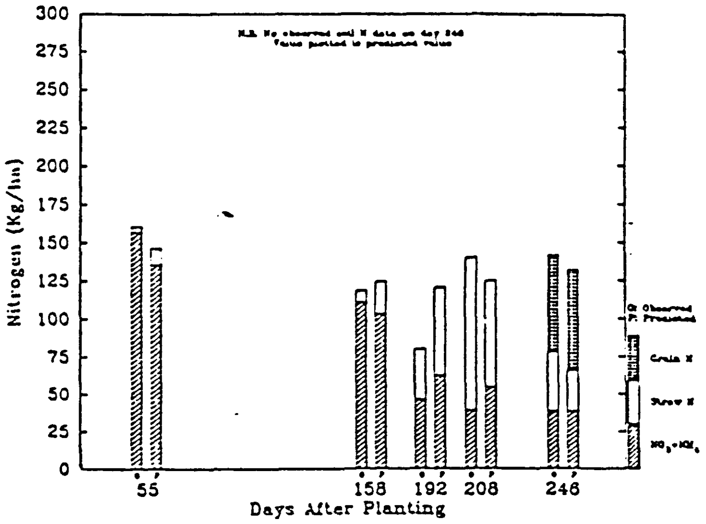


Figure 4.9. Continued.

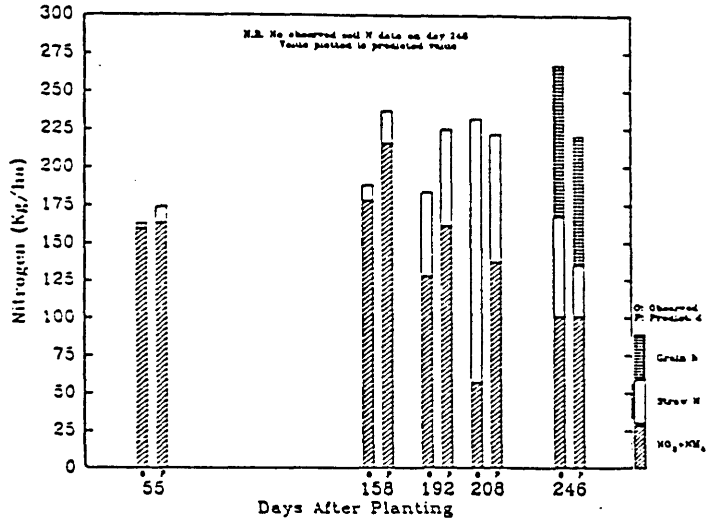
Manhattan Kansas 1981/82 0 Kg N/ha Dryland



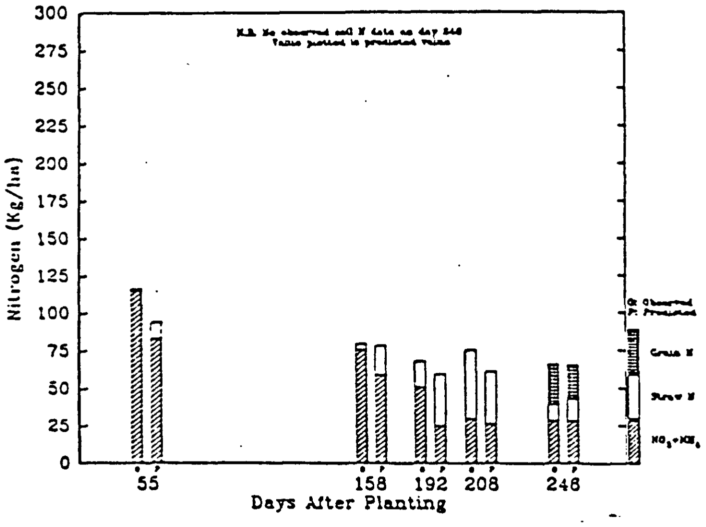
Manhattan Kansas 1981/82 60 Kg N/ha Dryland



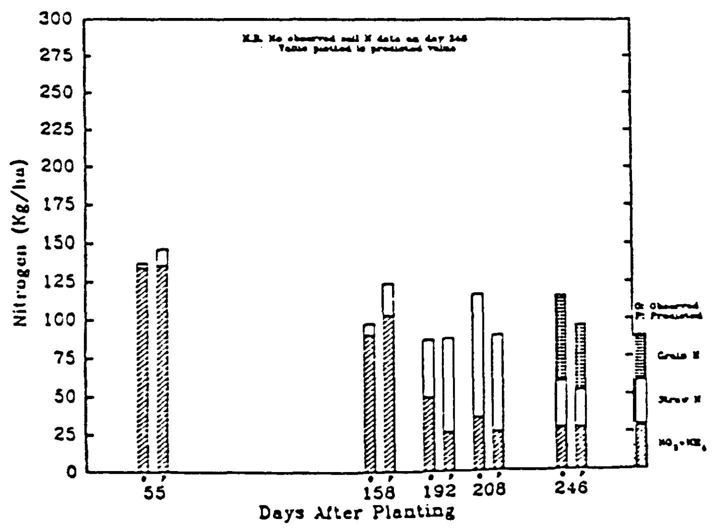
Manhattan Kansas 1981/82 180 Kg N/ha Dryland



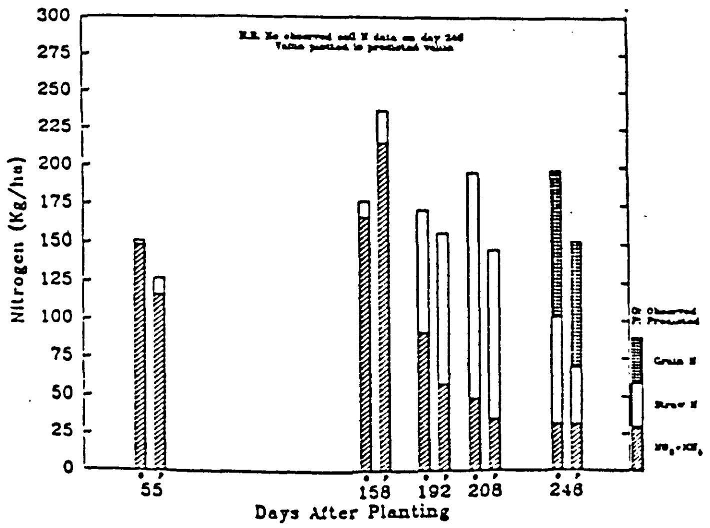
Manhattan Kansas 1981/82 0 Kg N/ha Irrigated



Manhattan Kansas 1981/82 60 Kg N/ha Irrigated



Manhattan Kansas 1981/82 180 Kg N/ha Irrigated



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