

# SOFTWARE

## GENCALC: Software to Facilitate the Use of Crop Models for Analyzing Field Experiments

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### ABSTRACT

A number of crop simulation models use as model inputs certain coefficients that account for differences among cultivars. These coefficients, often referred to as genotype coefficients, allow the models to simulate performance of diverse genotypes under different soil, weather, and management conditions. The models therefore can potentially be used to resolve the genotype  $\times$  environment interaction into underlying coefficients. GENCALC (Genotype Coefficient Calculator) is a software package that facilitates the calculation of these coefficients for use in existing crop models. In GENCALC, the coefficients for a genotype are estimated iteratively by running the appropriate crop model with model input data and approximate coefficients, comparing the model output with actual data, and then altering the coefficients until the simulated and measured values match. The coefficients are determined in a specified sequence, starting with those that relate to developmental aspects. GENCALC also allows for calculation of averages ( $\pm$  SD) for the coefficients determined from specific experiments. This facilitates the selection of coefficients with the lowest variability, which can then be stored in crop-specific database files. GENCALC comprises several programs and requires additional models and model input files, so a hard disk with  $\approx$  2 Mb free space is required. GENCALC will run on any IBM or IBM-compatible computer with DOS version 3.0 or later.

CROP MODELS could become valuable tools for use by researchers when analyzing data from field experiments. For such an application, though, models that account for the characteristics of different cultivars are required. Examples of such models are those of the CERES and GRO families. The CERES models encompass maize (*Zea mays* L.: Jones and Kiniry, 1986; Ritchie et al., 1989) and wheat (*Triticum aestivum* L.: Godwin et al., 1990a); GRO models include soybean [*Glycine max* (L.) Merr.: Jones et al., 1989], peanut (*Arachis hypogaea* L.: Boote et al., 1989) and dry bean (*Phaseolus vulgaris* L.: Hoogenboom et al., 1991). These models simulate crop growth, development and yield for specific genotypes, taking into account weather, soil water and N dynamics in the soil and crop in a mechanistic manner (Jones et al., 1990; Ritchie et al., 1990). Currently, the crop models do not simulate pest and disease effects nor the impact of nutrient shortages other than N (Godwin et al., 1990b).

In the CERES and GRO models, the ability to handle specific genotypes has been achieved by incorporating a file of coefficients that specify how a given genotype will respond to environmental factors such as minimum and maximum temperature, daylength, and soil

water and N contents, or that characterize certain aspects of the life cycle or morphology of the cultivar. These coefficients have been termed the genotype or genetic coefficients. Their nature, and the aspects covered by the coefficients used in the maize, soybean and wheat models have been described elsewhere (Hunt et al., 1990). Here it is sufficient to mention that the number of genotype coefficients varies from model to model, with the actual number varying from  $<10$  (e.g., CERES—Maize version 2.10) to  $>20$  (e.g., SOYGRO version 5.42).

Genotype coefficients may be determined in controlled environments or under field conditions. Since most model users do not have access to controlled environment facilities, however, most determinations will be made using field data. To help with this, we have developed and here report on a software package referred to as the Genotype Coefficient Calculator (GENCALC). The software enables users of the latest IBSNAT versions of the CERES and GRO models to estimate genotype coefficients from field data sets that contain the appropriate environmental and performance data for a particular genotype. The crop measurements that are needed to calculate genotype coefficients encompass the dates of key phenological stages such as emergence, flowering or anthesis and maturity, together with dry matter yield, harvest index and the standard yield components of the crop in question.

In GENCALC, the coefficients for a genotype are estimated iteratively by running the appropriate model with approximate coefficients, comparing the model output (e.g., dates of predicted events such as anthesis, pod appearance, etc.) to actual data, and then altering the genotype coefficient until the predicted and measured values match. The coefficients are determined in a preset sequence, with those that relate to phenological aspects being determined first.

### SPECIFICATIONS

GENCALC was developed to operate in standalone form (with appropriate models, of course) or as part of the software package known as DSSAT (Jones et al., 1990). The programs that comprise GENCALC were written in both Fortran and Basic. Compiled, executable files for these programs and sample model input files are included on the 3.5-inch (1.2 Mb) distribution diskettes; source code is available on request.

GENCALC version 3.0 will run on any IBM or IBM-compatible computer with DOS version 3.0 and later. A hard disk drive with  $\approx$  2 Mb free disk space is required. Total memory requirements depend on the specific model being used; in general, though, 600 K should be available. Color monitors are supported but not required. A printer is also not required, since all results are directed to the screen or to ASCII files. Because of the iterative nature of the calculations, however, a math co-processor is required. Even with a co-processor, the time taken

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for a GENCALC run can be considerable if a large number of coefficients are to be determined for a large number of experiments and treatments. For large data sets, therefore, a computer with a speed of 25 MHz or higher is recommended.

### Components and Documentation

GENCALC encompasses a number of components, depicted in flow chart form in Fig. 1. The executable programs and associated files specific to GENCALC are briefly described here.

#### GENCALC Programs

GENCALC.EXE is a *shell* program, written in Basic, that sets up the various control files, activates the overall control program, and runs the appropriate model. GCCALC.EXE is a *control* program, written in Fortran, that examines the model outputs and genotype coefficients. GCMEANS.EXE is an *averaging* program, written in Basic, that calculates means for coefficient values from individual experiments.

The Basic programs require a run-time module, BRUN45.EXE (included on the distribution diskette), which should be referenced in the DOS path statement.

#### GENCALC Files

DSSATPRO.FLE is a *profile* file that indicates the name and location on disk of programs and files that are used by GENCALC.

GCRULES.FLE is a file containing the rules that govern the sequence of genotype coefficient calculations for different crops. It is central to GENCALC operation. Its contents are copied to a temporary file (GCRULES.CTR) used during computation.

??COEFF.TMP and ENDPOINT.TMP are files generated internally at each new model run. The question marks (??) represent a two-character crop code, such as WH for wheat. The calculated genotype coefficient values are stored in ??COEFF.TMP; end-point information (simulated and measured values at completion) is stored in ENDPOINT.TMP for each coefficient. Information in these files can be displayed for perusal at the completion of a genotype coefficient calculation session.

??xxxxx0.CUL represents crop- and model-specific genetic coefficient files, which must include all genotypes included in an experiment. A user may need an ASCII file editor to enter a unique number and name into the file, along with an initial guess at the coefficient values, for any cultivar added to the file. A public domain editor, TED.COM, is available in GENCALC for making changes. The genotype coefficient files can be updated, at the user's discretion, during each session. These file names consist of a two-character crop code (??), the first five letters of the model name (xxxxx), and a final zero (0).

#### Other Files

In addition to the components above, the calculator requires a crop model output file, OVERVIEW.OUT, that contains a list of simulated and measured values for key variables, formatted and headed as described by Hunt et al. (1993).

The latest IBSNAT versions of the CERES and GRO models use the standard input and output file structures defined by Hunt et al. (1993). GENCALC was developed for use with these models; its use, however, is not restricted to them. GENCALC can be used with any crop model that conforms to the standards for genotype and overview files, and that uses the same run control procedures as the most recent IBSNAT models. Versions of the earlier IBSNAT maize, peanut, soybean and wheat models, modified to conform with these requirements, are included on the distribution diskette. Other models could be similarly modified; however, a model for a crop for which no IBSNAT equivalent exists would have to use a general or reference code (for *other crop*), rather than one specifically assigned (e.g., WH for wheat).

The permanent rules file (GCRULES.FLE), as set up for wheat

and maize, is depicted in Fig. 2. The number in the COEFF column of this file denotes the position in which the coefficient appears in the respective genotype file. Coefficients are not calculated in sequence with these position numbers, however, but in accordance with the row position in the rules file. Generally, developmental coefficients are dealt with first. Abbreviations for the coefficients, which correspond to those in the cultivar file, are presented in the name column. An index for the CERES and GRO models is provided in the file GENCOEFF.ABV, provided on the distribution diskette.

In GENCALC, it is possible to specify whether all coefficients are to be calculated, or only those related to development or growth. This is made possible by incorporating three rule sets for each crop. Rule Set 1 contains rules for the calculation of all coefficients, Rule Sets 2 and 3 are for developmental and growth coefficients, respectively.

In any GENCALC run, the iterative calculation begins with coefficients extracted from the genotype file and modified by the user if required. The first change in coefficient value is made using the value in the STEP column of the rules file. Subsequent changes are determined internally by linear extrapolation of the response to the previous change. The change in coefficient value, however, is limited to a maximum of 20%, to avoid the overshoot that can occur when the actual response is not linear. The maximum number of model runs allowed for the calculation of each coefficient is indicated in the column headed RMX. For most coefficients, the maximum number is set at nine model runs, and in most cases this has proven satisfactory. The MNCEF and MXCEF columns in the rules file indicate the acceptable minimum and maximum values for each coefficient, respectively. Acceptability of coefficients is determined by examining the difference between the measured and simulated data for a defined *target*. The target trait for each coefficient is indicated in the REF.NOS and REFERENCE TRAIT(S) columns. For each target, an acceptable difference is set in the rules file in the ERRMX column. If the minimum or maximum coefficient values are reached or the maximum run number is exceeded, the iterative calculation of the coefficient is terminated, even though the error may be unacceptable. A message indicating the reason for termination is assigned to the final iterated value (see later under program execution), and calculation for the next coefficient in the NAME column begins.

GENCALC requires the creation (if not already present) of a directory, C:\DSSAT3, and at one or more subdirectories named after the crop or crops in question. All required files are present on the distribution diskette in directories analogous to those needed on the hard disk.

#### Documentation

Documentation of GENCALC consists of a 10-page user's guide that describes the components of GENCALC, the installation procedures, and step-by-step instructions to cover the basics of operation. Crop model documentation is not distributed with GENCALC, as it can be obtained along with the required model from the model developers.

### PROGRAM EXECUTION

The calculation of genotype coefficients with the calculator requires data sets complete with crop, weather, and soil data for the genotype in question, with appropriate initial genetic coefficient estimates in the cultivar file. The data sets must be placed into a directory allocated for crop model input files (e.g., wheat data into C:\DSSAT3\WHEAT). Once these are set up, GENCALC can be accessed directly or through the DSSAT 3.0 shell. The actual calculation of the coefficients within GENCALC, however, requires several user-specified instructions.

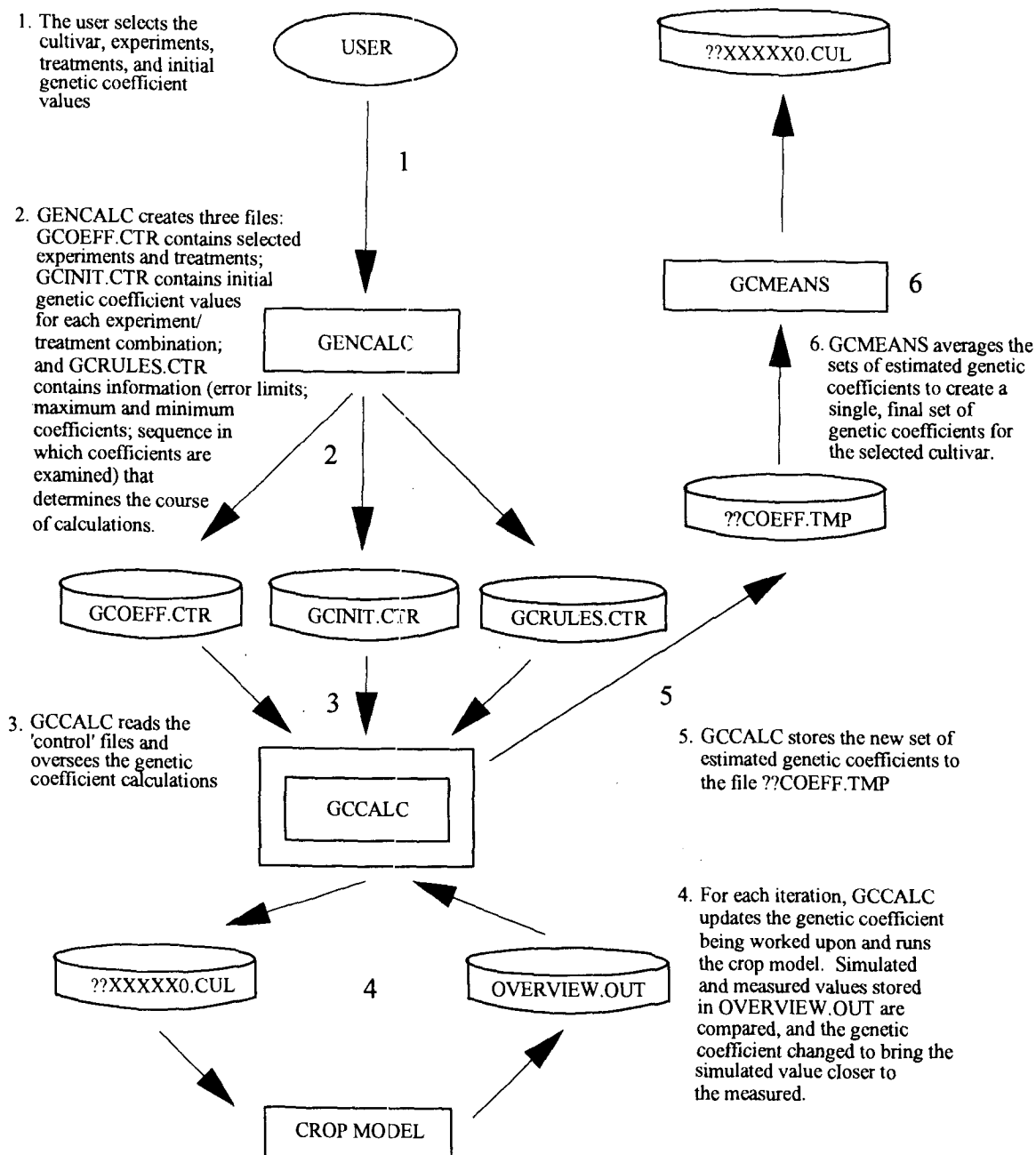


Fig. 1. Flow chart for GENCALC (the Genotype Coefficient Calculator).

GENCALC prompts the user for these instructions. The procedure is described below to highlight the options that are available, with sample screens for a wheat cultivar, Katepwa.

The first step is to choose from two possible options: (i) calculate coefficients for specific experiments and treatments; or (ii) calculate averages from coefficients determined for specific experiments and treatments in previous sessions. If the first objective is selected, then the user selects the crop for which genotype coefficients are to be calculated. Once this is done, the GCSHELL program determines which genotypes are present and lists those available for analysis (Fig. 3a). Coefficients taken from the cultivar file of the crop concerned are then

displayed for the selected genotype. These can be accepted for the initial model run of the calculation (Fig. 3b), or modified at user discretion. Abbreviations used to reference a particular coefficient are taken from the cultivar file of the crop in question.

The next step is to choose whether the development, growth, or both development and growth coefficients are to be calculated. The choice of the appropriate coefficient set depends on the particular application for which coefficients are being calculated. Generally it is more efficient to determine the development coefficients before proceeding to the growth aspects. Following coefficient selection, lists of experiments and treatments that include the selected genotype will be displayed for se-

## GENOTYPE COEFFICIENT RULES FILE

COEFF	NAME	REF.NOS	STEP	ERRMX	RMX	MNCEF	MXCEF	REFERENCE TRAIT(S)
<b>*WHCER20 1 WHEAT ALL COEFFICIENTS</b>								
3	DESP(P1D)	1/00*00	0.2	1.0	9	0.0	9.9	ANTHESIS DATE
2	DESV(P1V)	1/00*00	0.2	1.0	9	0.0	9.9	ANTHESIS DATE
1	DUGF(P5)	2/00*00	2.0	1.0	9	-9.9	59.9	MATURITY DATE
7	BIOM	8/00*00	0.1	100.0	9	0.4	19.5	BIOMASS
4	GNUM(G1)	5/00*00	0.5	100.0	9	0.0	59.9	GR M <sup>2</sup>
6	GNUS(G3)	8/00*00	0.5	2.0	9	-9.0	59.9	GR SPIKE <sup>1</sup>
5	GGRO(G2)	4/00*00	0.5	2.0	9	-9.9	19.9	GRAIN WEIGHT
<b>*WHCER20 2 WHEAT DEVELOPMENT COEFFICIENTS ONLY</b>								
3	DESP(P1D)	1/00*00	0.2	1.0	9	-1.0	9.9	ANTHESIS DATE
2	DESV(P1V)	1/00*00	0.2	1.0	9	-1.0	9.9	ANTHESIS DATE
1	DUGF(P5)	2/00*00	2.0	1.0	9	-9.9	59.9	MATURITY DATE
<b>*WHCER20 3 WHEAT GROWTH COEFFICIENTS ONLY</b>								
7	BIOM	8/00*00	0.1	100.0	9	0.4	19.5	BIOMASS
4	GNUM(G1)	5/00*00	0.5	100.0	9	0.0	59.9	GR M <sup>2</sup>
6	GNUS(G3)	8/00*00	0.5	2.0	9	-9.0	59.9	GR SPIKE <sup>1</sup>
5	GGRO(G2)	4/00*00	0.5	2.0	9	-9.9	19.9	GRAIN WEIGHT
<b>*MZCER20 1 MAIZE ALL COEFFICIENTS</b>								
3	DESP(P2)	1/00*00	1.0	1.0	9	0.0	3.0	SILKING DATE
1	DUJU(P1)	1/00*00	20.0	1.0	9	0.0	500.0	SILKING DATE
2	DUGF(P5)	2/00*00	50.0	1.0	9	500.0	1500.0	MATURITY DATE
6	BIOM	8/00*00	0.1	100.0	9	-0.1	19.5	BIOMASS
4	GNUM(G2)	5/00*00	100.0	100.0	9	200.0	1600.0	GRAINS M <sup>2</sup>
5	GGRO(G3)	4/00*00	0.5	.02	9	1.0	12.0	GRAIN WEIGHT
<b>*MZCER20 2 MAIZE DEVELOPMENT COEFFICIENTS ONLY</b>								
3	DESP(P2)	1/00*00	1.0	1.0	9	0.0	3.0	SILKING DATE
1	DUJU(P1)	1/00*00	20.0	1.0	9	0.0	500.0	SILKING DATE
2	DUGF(P5)	2/00*00	50.0	1.0	9	500.0	1500.0	MATURITY DATE
<b>*MZCER20 3 MAIZE GROWTH COEFFICIENTS ONLY</b>								
6	BIOM	8/00*00	0.1	100.0	9	-0.1	19.5	BIOMASS
4	GNUM(G2)	5/00*00	100.0	100.0	9	200.0	1600.0	GRAINS M <sup>2</sup>
5	GGRO(G3)	4/00*00	0.5	.02	9	1.0	12.0	GRAIN WEIGHT

NB. COEFF=COEFFICIENT (WITH NUMBERS IN THE FIRST TWO COLUMNS REPRESENTING THE SEQUENCE IN THE MODEL INPUT GENETICS FILE); REF=REFERENCE TRAIT; STEP=STEP TO INCREMENT COEFFICIENT; ERRMX=ERROR LIMIT FOR ACCEPTANCE OF ESTIMATE; RMX=MAXIMUM NUMBER OF RUNS; MNCEF=MINIMUM VALUE FOR COEFFICIENT; MXCEF=MAXIMUM VALUE FOR COEFFICIENT.

Fig. 2. The rules file used for the calculation of genotype coefficients of wheat and maize in GENCALC.

lection or rejection (Fig. 3c). Any number of experiments and treatments can be specified. Selection of several experiments and treatments at this point is helpful, however, in the calculation of mean genotype coefficients (see below).

Upon completion of the above steps, the calculator runs the appropriate crop model and displays data indicating the goodness-of-fit between simulated and measured data (Fig. 3d). End-point information (simulated and measured data for the target trait) is stored for viewing at the end of calculations, and final coefficient values are placed in ??COEFF.TMP for storage, viewing, and averaging if desired. A screen allowing access to an editor of choice appears at the end of calculations. The editor provides access to the files of final coefficient and end-point information.

While viewing the final coefficients, attention must be paid to the letter codes, such as *U*, *M*, or *R*, that GENCALC may assign to each of the calculated coefficients. A *U* immediately following the numerical value indicates that the particular coefficient was not determined during calculation, as specified by the user in the coefficient selection step. An *M* after the numerical value indicates that the calculated coefficient reached the maximum or minimum value defined in the GCRULES file. In this case, depending on whether the coefficient was near the minimum or maximum, the rules file must be edited to reduce or increase the MNCEF or MXCEF for the rules set. This can be done from within GENCALC in the coefficient selection step. If the maximum number of runs specified in the GCRULES file was reached before an acceptable end point was reached, the numerical value for the coefficient in question will have an *R* associated with it. If so, in the initial values selection step, the coefficient must be

increased by  $\approx 30\%$  if the simulated was less than the measured, or decreased a like amount if the inverse.

The data accumulated for individual runs in the ??COEFF.TMP file can be summarized by accessing the averages option from the main screen. Choosing this option will bring up a list of genotypes for which genotype coefficients were calculated previously and are still available. Selection of a genotype will lead to the display of a list of coefficients that were calculated in previous experiment/treatment runs. Each of these runs is assigned a number in the listing, with calculations made with the same initial values having the same run number.

Once a run number is chosen, average coefficients are calculated, along with their respective coefficients of variation. These values are displayed together with values currently in the cultivar file. Coefficients that were not fitted well are not displayed. Additional runs may be chosen. Once the selection of one or more runs is completed, a table of standard deviations for coefficients from all chosen runs is displayed. From this table a run must be chosen—probably the one with the lowest standard deviation for a number of coefficients. If required, values for the chosen run can then replace the old values in the cultivar coefficient file.

Following the satisfactory calculation of the coefficients for one cultivar, the user may select another cultivar of the same crop, or change to another crop to set up another sequence of calculations.

## AGRONOMIC APPLICATIONS

Crop improvement programs traditionally evaluate genotypes in multienvironment, multiyear trials, the variation commonly being analyzed using the model

$$P = G + E + GE$$

where *P*, *G*, *E*, and *GE* refer to phenotypic, genotypic, environmental and genotype  $\times$  environmental effects, respectively (Shorter et al., 1991). In this model, the *GE* term combines all the specific genotypic responses to the environment into one parameter (Blum, 1984) thus providing little insight into the biological significance of the genotype  $\times$  environment interactions. Further utility could be obtained from the data if the overall *GE* term could be broken down into the various ecophysiological characteristics that determine response to environmental factors. The genotype coefficients used by various crop models attempt to capture the essence of these physiological characteristics. They can be determined by using those models that best express current understanding of genotype  $\times$  environment interactions. The use of a model in this context has generally been rather cumbersome and tedious and unlikely to be attempted in routine work; GENCALC, however, aids use in such a mode. GENCALC can thus be viewed as a tool to bring together inputs from plant breeding, crop physiology, and crop modeling to aid in the decision making processes in plant breeding and agronomy. Examples of potential uses are for decisions on the release of new cultivars from a breeding program, or for decisions on a new management technique for an existing and/or new cultivar. GENCALC, as a software package that facilitates the analysis of field experiments in terms of those coefficients that underlie *G*  $\times$  *E* interaction, could thus play

## a) Listing of available genotypes

G.C. CALCULATOR - INDIVIDUAL

VERSION 3.0

CROP: Wheat	
No	Name
1	WARED
2	KATEPWA
3	ANZA
Enter NUMBER to select genotype, or blank to exit --->	

## b) Listing of genotype coefficients

G.C. CALCULATOR - INDIVIDUAL

VERSION 3.0

CROP: Wheat							
Current coefficients are:							
DUGF	DESV	DESP	GNUM	GGRO	GNUS	BIOM	LFAP
1	2	3	4	5	6	7	8
456.	.000	.000	42.5	1.56	2.93	1.29	68.0
Use these for initial run?							
Press: Y or N							

## c) Presentation of available experiments

G.C. CALCULATOR - INDIVIDUAL

VERSION 3.0

CROP: Wheat
The selected genotype was included in experiment: ONSW910U
Accept this experiment?
Press: Y or N

## d) Presentation of the status of calculations

G.C. CALCULATOR - INDIVIDUAL

VERSION 3.0

Crop	:WH
Experiment	:ONSW910U
Treatment #	:4
Treatment run #	:12
Coefficient	:GNUS(G3)
Coeff.run #	:7
Computed	:23.280
Measured	:29.370
Old coef. value	: 5.930
New coef. value	: 6.430

Fig. 3. Some sample screens from GENCALC.

an important role in agronomy as well as have use in model development.

## AVAILABILITY

GENCALC is available from the Department of Crop Science, University of Guelph, ON, Canada N1G 2W1, or from the IBSNAT Project, University of Hawaii at Manoa, Department of Agronomy and Soil Science, 2500 Dole St., Room 22, Honolulu, HI 96822. The price is \$50 (U.S.) to cover the cost of materials and shipping. Inquiries should be addressed to Dr. L.A. Hunt at the Canadian address.

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