

CHAPTER 3

MATERIALS AND METHODS

3.1 Site selection

The research focused an effort in the deepwater rice area of Prachin Buri and Chachoengsao provinces in the eastern plain of Bangkok. The 14 sub districts (Tambons) were selected including of Ban Sang, Bang Kham, Bang Krabao, Bang Pla Ra, Bang Phluang, Bang Taen, Bang Toei, Bang Yang, Bang Decha, Dong Kratong Yam, Krathum Paeo, Pai Cha Lued, and Tha Ngarm of Prachin Buri province and Bang Kra Chet of Chachoengsao province. The study area was located between longitude of $101^{\circ} 08'$ and $101^{\circ} 27'$ E and latitude of $13^{\circ} 48'$ and $14^{\circ} 03'$ N (Figure 2). It was situated on a flat low land topography, with an averaged elevation of two meter above mean sea level. The research area was a part of Bang Pakong river basin, Nakhon Nayok sub watershed of the Bang Pakong river basin, and Prachin Buri river basins (Figure 3). Before the construction of Khun Dan Prakanchol dam and irrigation systems, farmers practiced deepwater rice production, which began in April and harvests in December. The irrigation systems enabled farmers, in the lower part of the area, transformed from the DWR to FDR production system during the early 1990s (Figure 4).

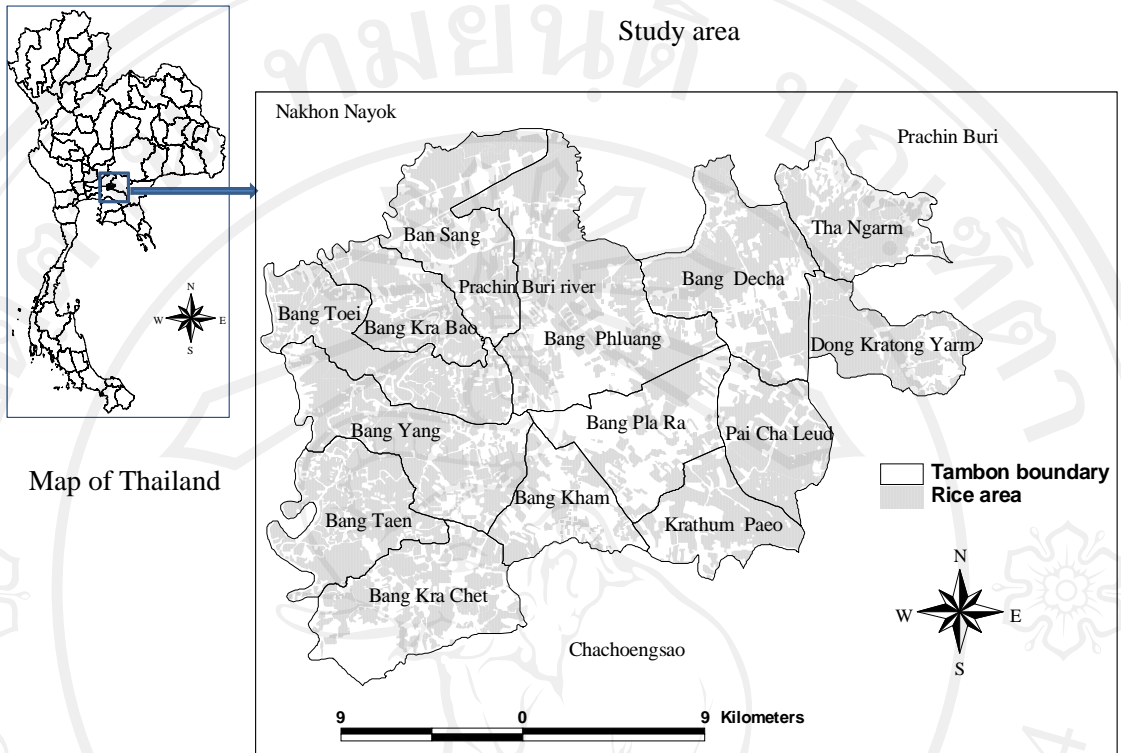


Figure 2 Map of the study area in 14 Tambons of Prachin Buri and Chachoengsao provinces, Thailand, 2009.

Source: Land Development Department, Thailand

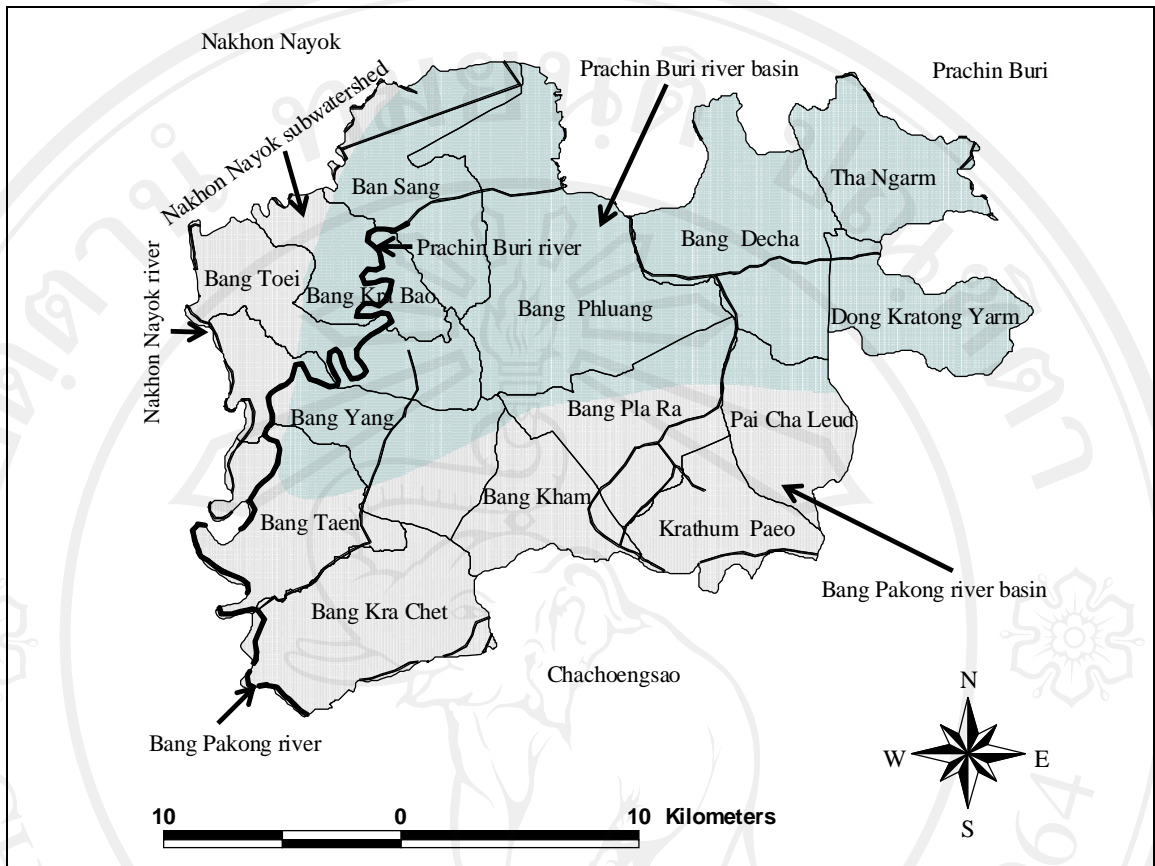


Figure 3 Study areas within the Bang Pakong and Prachin Buri river basins
Source: Land Development Department, Thailand

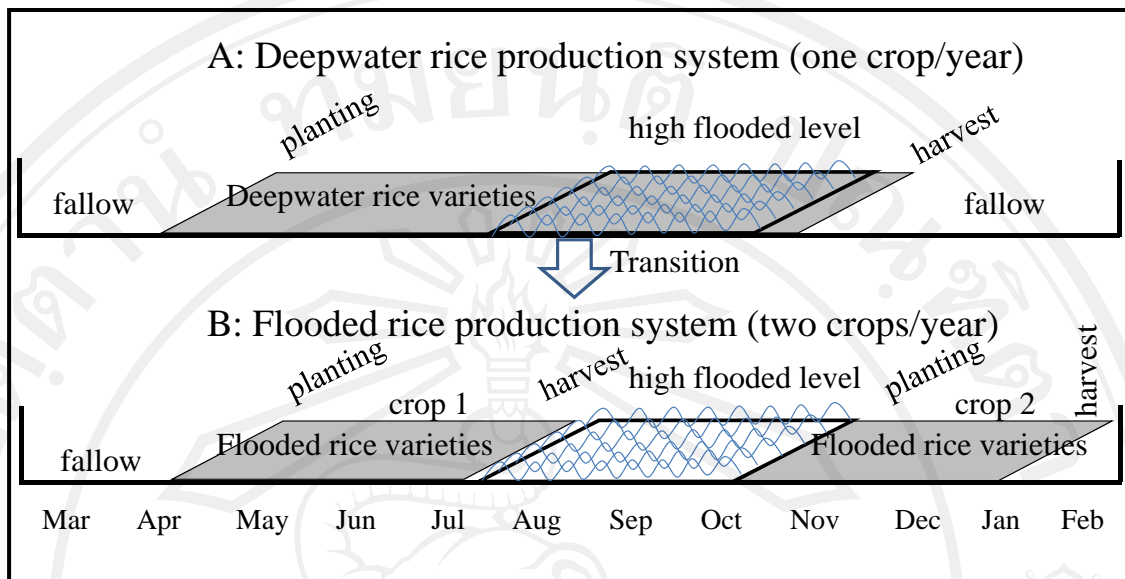


Figure 4 Transitional phase of deepwater rice production to flooded rice production system, A: Deepwater rice production system, B: Flooded rice production system.

3.2 Secondary data collection

Secondary data sets had been collected from three local government organizations to establish and gain better understandings of deepwater rice production system in the area. Administrative boundary and rice production area statistics were collected from Land Development Department, Ministry of Agriculture and Cooperatives. Number and locations of the villages and number of population were collected from the office of Tambon Administrative Organizations (TAOs) in the study area. Weather data was provided by the Prachin Buri Meteorology station, Meteorology Department.

3.3 Farmer interview

Data collection from 14 TAOs showed a total of 12,367 households (Table 3) in 128 villages of the study area. The research applied the Yamane formula (Yamane, 1967) to calculate a reasonable sample size as follows;

$$n = \frac{N}{1+N(e)^2} \quad (1)$$

where: n = number of households to be interviewed

N = total number of households in the study site

e = precision level (.05)

According to the formula, a minimum of 388 households was required to obtain reasonable data set for this study. With support from TAOs and local farmer groups, however, a total of 402 farm-households were interviewed, using a closed-ended formal questionnaire (Appendix A). The questions were designed to provide understanding of characteristics of rice farms, factors influencing farmer's decision to transform to FDR, and farmer's sources of information regarding selecting planting dates, appropriate rice variety, and suitable chemical fertilizer management. Descriptive statistics and simple comparison of means and standard deviation support our data analysis and synthesis.

Table 3 Name of 14 Sub-districts, number of villages, household, population, total area and rice area of the study sites in the Prachin Buri and Chachoengsao province, Thailand for 2009.

| <i>Province</i> | <i>District</i> | <i>Tambon</i> | <i>Village #¹</i> | <i>Household¹ No.</i> | <i>Population¹</i> | <i>Total Area² (ha)</i> | <i>Rice area (ha)</i> | <i>Rice area (% of total)</i> |
|-----------------|-----------------|----------------|------------------------------|--------------------------------------|-------------------------------|--|---------------------------|-----------------------------------|
| Prachin Buri | Ban Sang | Ban Sang | 11 | 775 | 3,016 | 4,537 | 2,947 | 65 |
| | | Bang Kham | 5 | 563 | 1,518 | 2,737 | 1,142 | 42 |
| | | Bang Krabao | 9 | 688 | 2,497 | 2,685 | 1,955 | 73 |
| | | Bang Pla Ra | 8 | 1,527 | 5,506 | 4,046 | 1,536 | 38 |
| | | Bang Phluang | 11 | 1,257 | 5,901 | 7,858 | 4,920 | 63 |
| | | Bang Taen | 13 | 1,095 | 4,305 | 3,838 | 2,871 | 75 |
| | | Bang Toei | 10 | 536 | 2,077 | 3,959 | 3,019 | 76 |
| | | Bang Yang | 13 | 1,030 | 4,561 | 4,934 | 3,369 | 68 |
| | | Krathum Paeo | 7 | 463 | 1,523 | 2,749 | 1,847 | 67 |
| | Muang | Bang Decha | 9 | 625 | 3,400 | 5,351 | 3,662 | 68 |
| | | Tha Ngam | 12 | 933 | 4,696 | 3,187 | 2,047 | 64 |
| | | Sri Maha Phote | Dong Kratong Yam | 7 | 943 | 4,121 | 2,888 | 2,241 |
| | Sri Mohosote | Pai cha lued | 4 | 904 | 3,147 | 2,953 | 2,168 | 73 |
| | Chachoengsao | Bang Kla | Bang Kra Chet | 9 | 1,028 | 4,601 | 4,980 | 2,442 |
| Total | | | 128 | 12,367 | 50,869 | 56,702 | 36,165 | |
| Average | | | | | | | | 64 |

Source: ¹ 14 Tambon Administrative Organizations, PrachinBuri and Chachoengsao province.

² Land Development Department, Thailand.

3.4 Field experiments

Field experiments were conducted at Bang Taen His Majesty Private Development Project, Bansang, Prachin Buri, Thailand, located at a latitude of $13^{\circ} 52'$ N, a longitude of $101^{\circ} 09'$ E with an elevation of two meters above mean sea level. Prior to land preparation, composite soil samples were collected at four different soil depths at 15 cm interval from 0 to 60 cm (Hoogenboom *et al.*, 1999). Four soil layers of 0-15, 15-30, 30-45, and 45-60 cm depth in each sampling spot were done, a total of 12 soil samples were collected. Three sampling spots for taking soil samples and the total of 10 samples of previous crop biomass were taken. The previous crop of experimental field was rice crop. However, the collected previous crop aboveground biomass consisted of rice straw, weed and rice seedlings from the fallen grains during harvest of the previous rice crop. The total nitrogen, available phosphorus and extractable potassium were analyzed by using Micro Kjeldahl method, Bray II method and Neutral ammonium acetate method, respectively (Bray and Kurtz, 1945; Jackson, 1965; Pratt, 1965). Laboratory procedure was supported by Pathum Thani Rice Research Center.

There were two experiments conducting during 2009–2010. The first experiment was “The Effect of Planting Date and Variety on Flooded Rice Production in the Deepwater Area of Thailand” and the second experiment was “The Effects of Nitrogen Fertilizer Management and Variety on Flooded Rice Production in the Deepwater Area of Thailand”. Both experiments were conducted in early rainy season (ERS) and dry season (DS) crops.

The experimental design of the first experiment was split plot in a randomized complete block with four replications. Planting date (PD) was the main plot and the

variety (V) was the sub-plot and randomized within each planting date. There were a total of four planting dates and three rice varieties. For both the ERS and the DS cropping seasons, the same three rice varieties were grown which consisted of Chai Nat 1 (CNT1), Pathum Thani 1 (PTT1) and Pitsanulok 2 (PSL2). The first planting date (PD1) of the ERS experiment was started on May 20 followed by PD2 on June 3, PD3 on June 24, and PD4 on July 1, 2009. The crop for the first planting date was harvested on September 17, and the crop for the last planting date was harvested on October 21, 2009. The DS crop started in November. The first crop PD1 was planted on November 9, followed by November 23, December 8, and December 21, 2009 for PD2, PD3, and PD4, respectively. The first harvest for the DS crop started on February 26, 2010, and on April 15, 2010 for PD4 crop (Table 4).

Land preparation was conducted with a seven disk implement tractor for the first plowing and a hand rototiller for the second plowing, within one week after the first plowing and followed by harrowing. Following land preparation, rice seedlings were transplanted at a spacing of 20 x 20 cm with three seedlings per hill. The area of the main plot was 7.0 x 8.8 m with three sub plots of 7.0 x 2.8 m (Figure 5). The border between each main plot was one meter. Each sub plot contained 15 rows with 36 hills per row. Continuous flooding was maintained at the depth of 10 cm. There were two applications of chemical fertilizer; the first application was applied at a rate of 30 kg N and 36 kg P₂O₅ ha⁻¹ at one week after transplanting and the second application was

Table 4 Seeding, transplanting and harvesting dates of three rice varieties in early rainy season and dry season crop of flooded rice production in deepwater area, Prachin Buri, Thailand. 2009-2010

| <i>Planting Date</i> | <i>Seeding date</i> | <i>Transplanting date</i> | <i>Harvesting date</i> | | |
|----------------------|---------------------|---------------------------|------------------------|--------------|--------------|
| | | | <i>CNT1</i> | <i>PTT1</i> | <i>PSL2</i> |
| Early rainy season | | | | | |
| PD1 | May 20, 2009 | Jun 19, 2009 | Sep 23, 2009 | Sep 21, 2009 | Sep 17, 2009 |
| PD2 | Jun 3, 2009 | Jul 2, 2009 | Oct 2, 2009 | Sep 30, 2009 | Sep 26, 2009 |
| PD3 | Jun 24, 2009 | Jul 16, 2009 | Oct 14, 2009 | Oct 21, 2009 | Oct 14, 2009 |
| PD4 | Jul 1, 2009 | Jul 23, 2009 | Oct 24, 2009 | Oct 26, 2009 | Oct 21, 2009 |
| Dry season | | | | | |
| PD1 | Nov 9, 2009 | Dec 9, 2009 | Feb 26, 2010 | Mar 8, 2010 | Feb 26, 2010 |
| PD2 | Nov 23, 2009 | Dec 21, 2009 | Mar 8, 2010 | Mar 21, 2010 | Mar 8, 2010 |
| PD3 | Dec 8, 2009 | Jan 7, 2010 | Mar 24, 2010 | Apr 7, 2010 | Mar 24, 2010 |
| PD4 | Dec 21, 2009 | Jan 18, 2010 | Apr 15, 2010 | Apr 19, 2010 | Apr 15, 2010 |

applied at a rate of 29 kg N ha⁻¹ at panicle initiation (PI) stage (Department of Agriculture, 2004a).

The experimental design of the second experiment was also a split plot in randomizing complete block with four replications. Four fertilizer managements (Table 5) and three flooded rice varieties were the main plots and sub plots, respectively. Three rice varieties were Chai Nat 1 (CNT1), Pathum Thani 1 (PTT1) and Pitsanulok 2 (PSL2). Main plot size was 7.0 x 6.4 m. Each main plot consisted of three sub plots of 7.0 x 2.0 m (Figure 6). The main plots were separated by one meter spacing apart with a 30 cm bund height to control water and fertilizer movement. For ERS crop started to prepare seedbed on May 20, transplanting on June 19, and harvested on September 17 - 23, 2009, depending on varieties. The DS crop started to prepare seed bed on November 9, transplanting on December 9, 2009, and harvested between February 26, and March 8, 2010.

Experimental unit layout of harvested area for biomass data collection

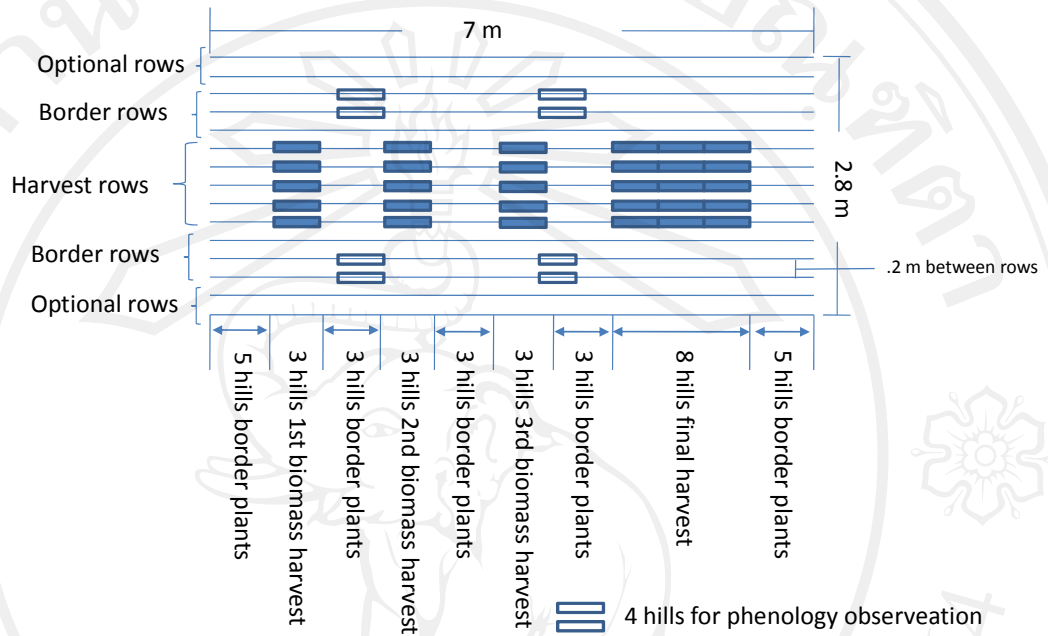


Figure 5 Plot layout for sampling collection in sub plot of the effects of planting date and variety on flooded rice production in the deepwater area of Thailand (Hoogenboom *et al.*, 1999).

Experimental unit layout of harvested area for biomass data collection

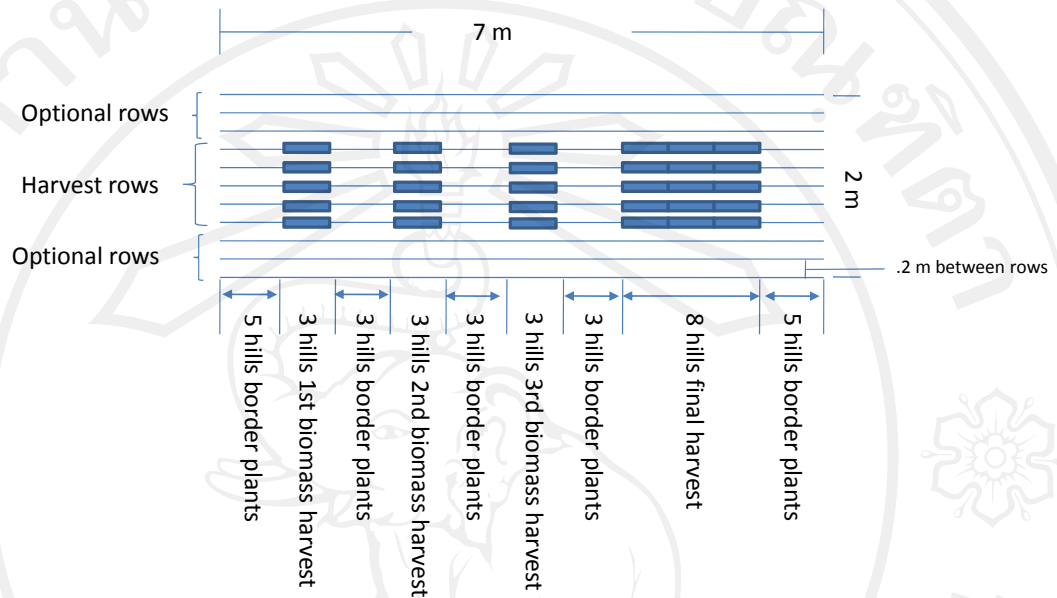


Figure 6 Plot layout for sampling collection in sub plot of the effects of nitrogen fertilizer management and variety on flooded rice production in the deepwater area of Thailand (Hoogenboom *et al.*, 1999).

Four main plots of fertilizer managements were:

- F1: No fertilizer application
- F2: Farmer application rate (application rate defined by collecting data from the farmers surround the area of experimental site)
- F3: Chemical fertilizer application base on Leaf Color Chart (LCC) technique with board casting (BC) (Furuya, 1987; Peng *et al.*, 1996).
- F4: Leaf Color Chart (LCC) technique with deep placement (DP) (Bowen, 2005; Furuya, 1987; Peng *et al.*, 1996)

Three popular recommended flooded rice varieties for the sub plots were Chai Nat 1 (CNT1), Pathum Thani 1 (PTT1) and Pitsanulok 2 (PSL2). Each sub plot contained 11 rows of 36 rice hills. Continuous flooding at a depth of 10 cm was maintained throughout the growing season. For fertilizer treatments, twice applications of chemical fertilizer were applied. The first application was made at one week after transplanting and the second application was made at the panicle initiation (PI) stage.

Fertilizer application rate of F2 was the rate that farmers normally used, while F3 and F4 were defined by LCC technique (Furuya, 1987; Peng *et al.*, 1996) (Table 5). It's the same rate for F3 and F4 treatment, but it differed in the mode of application. Broadcasting and deep placement techniques were the application mode for F3 and F4 treatment, respectively. Deep placement was an application technique by inserting a mud ball containing fertilizer into the rice root zone at a depth of 5 cm (Bowen, 2005).

Table 5 Four main plots of fertilizer management in the effect of fertilizer management and variety on flooded rice production in the deepwater area, Prachin Buri, Thailand 2009 – 2010

| <i>Main plot (Fertilizer management)</i> | <i>Application rates</i> | | <i>Method of application</i> |
|--|--|--|----------------------------------|
| | First application (kg N, P ₂ O ₅ ha ⁻¹) | Second application (kg N ha ⁻¹) | |
| F1 | 0, 0 | 0 | - |
| F2 | 35, 44 | 43 | Broadcasting |
| F3 | 30, 36 | 29 | Broadcasting |
| F4 | 30, 36 | 29 | Deep placement |

3.4.1 Data collection

A rice plant had three major developmental phases including the vegetative phase, the reproductive phase and the ripening phase (Department of Agriculture, 2004b; Kunnoot, 2006). The vegetative phase covered the period from germination to panicle initiation. The reproductive phase covered the period from panicle initiation to flowering phase and the ripening phase covered the period from flowering to maturity. The developmental stages and associated dates were monitored including the panicle initiation date, flowering date, the milky date and the maturity or harvesting date (Figure 7). The panicle initiation date was monitored daily from 50 days after planting until appearance of the panicle primordium. For the other developmental stages a five day interval was used for monitoring. Biomass samples for growth analysis were collected throughout the growing season (Hoogenboom *et al.*, 1999). Biomass samples were collected five times, including at the seedling stage (a stage during the vegetative phase), panicle initiation stage, flowering stage, milky stage and maturing stage (Department of Agriculture, 2004b). One hundred plants for each variety were collected at the seedling stage before transplanting. For the panicle initiation stage, flowering stage and milky stage, the numbers of 15 hills per plot were

sampled. At the final harvest, the numbers of 25 hills were sampled for biomass, yield and yield component evaluation. The individual stem, leaf and panicle components of the sampled rice hills were separated and dried in a hot air oven at 75°C for 72 hours until constant weight and then weighed for further growth analysis.

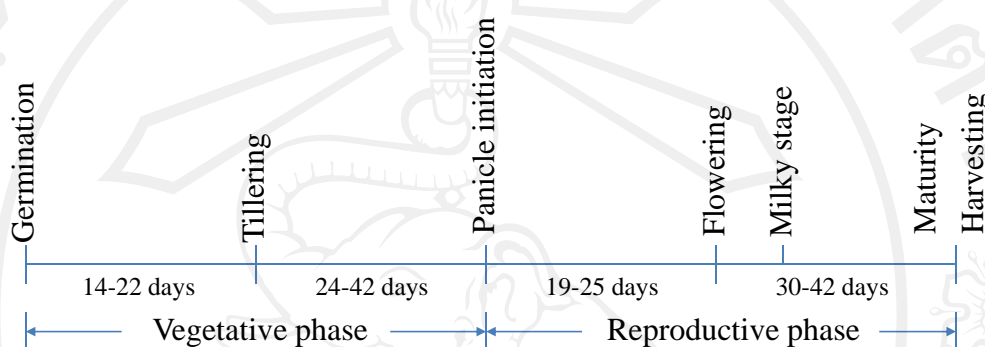


Figure 7 Development phases of rice plant from germination to harvest (variable time 0-25 day dependent upon variety)

3.4.2 Rice development phases

Development phases of four hills rice plant in each sub-plot were also monitored throughout the growing season. Four development phases were recorded including panicle initiation stage, flowering stage, milky stage and maturing or harvesting stage (Department of Agriculture, 2004b). The panicle initiation was the initiation of the panicle primordia at the tip of the growing shoot to begin the reproductive phase. Flowering began when anthers protruded from the spikelets and then fertilization took place. The date of flowering was the date at which 50% of rice plants in specified hills flower. Milky stage was stage that the grain had begun to fill with a milky material. The grain starts to fill with a white milky liquid, which could be squeezed out by pressing the grain between the fingers. Mature grain or harvesting

stage was the stage at individual grain was fully developed, hard, and husked had turned to yellow at ninety to hundred percent of the total grain of the specified hills.

3.4.3 Rice plant nitrogen

Nitrogen in the stem and leaf biomass under different fertilizer management of ERS crop were analyzed to measure total nitrogen uptake using Micro Kjeldahl method (Jackson, 1965; Pratt, 1965). Four stages of three rice cultivars under four fertilizer managements were collected for total nitrogen analysis in laboratory. A total of 96 plant samples were taken for nitrogen uptake measurement.

3.5 Model calibration and evaluation

The following data sets were collected for model calibration and evaluation, included rice crop management, daily weather data set, soil environments and primary genotype characteristics as shown below (Hunt and Boote, 2002).

Data sets for model operation consist of:

- Description of field experiment site: latitude, longitude, elevation and elevation from mean sea level.
- Weather data: daily maximum and minimum air temperature, and precipitation (provided by the Prachin Buri Meteorology Station, Meteorology Department, Thailand), solar radiation on daily basis was calculated base on maximum and minimum temperature (Jintrawet *et al.*, 2002; Hunt *et al.*, 1998)
- Soil data: soil analysis by layer, soil bulk density, organic carbon, organic

- Initial condition: biomass of previous crop
- Crop managements: rice cultivar name, planting date, planting method, spacing and plant population
- Irrigation and water management
- Fertilizer management: formula of fertilizer, time and amount of application and method of application
- Rice crop performance: date of planting, panicle initiation, flowering, milky and harvesting date, yield and yield components, and percentage of leaf N in crop biomass.

3.5.1 Field experiments for model calibration and evaluation

The data sets from the both field experiments named “The Effect of Planting Date and Variety on Flooded Rice Production in the Deepwater Area of Thailand” and “The Effects of Nitrogen Fertilizer Management and Variety on Flooded Rice Production in the Deepwater Area of Thailand” conducting in ERS and DS were used to calibrate and evaluate the CSM-CERES-Rice Model. The experimental detail was explained in the section 3.4 and the data collection mentioned in the section 3.4.1 to 3.4.3.

3.5.2 Preparation of input files for CSM-CERES-Rice model

Five input files were prepared for the CSM-CERES-Rice model, including FileX, FileA, FileT, Soil file, and Weather file (Appendix C). FileX or management file indicated the environment of the field condition, field management, treatments in the experiment, and simulation option. The existing field environment indicated weather data, soil property, and initial condition of the field. The major part of FileX

was crop production management. This part defined rice cultivar, planting detail, irrigation, fertilizer application (organic and inorganic), tillage, harvest and chemical application. Simulation control section served as model calculation control part. It pointed out when to start simulation, what to calculate, what method of calculation should be used under particular management. The output could also be framed under simulation option part. Treatment part was a combination of environment, management and simulation option part.

FileA and FileT stored the observed data of four field experiments, include rice growth, rice phenology, yield, and yield components data. FileA comprised the details of each treatment at the final harvest period of the experiment, while FileT provided the details of growth analysis of the crop during its life cycle on different phenological stages of each treatment.

Soil file contained physical and chemical soil characteristics of the field experimental plot. Soil composite samples were collected from four soil layers as explained earlier. Most of rice roots were in the first layer. Soil pH, organic matter, total N, available P, extractable K, and soil bulk density were analyzed. Biomass of previous crop was also collected at the same time of taking soil samples. Soil and previous crop biomass sampling was performed seven days before making plough.

The amount of previous crop biomass in the experiment field was $3,725 \text{ kg ha}^{-1}$. Analyzed data of soil samples and previous crop biomass were used to create the soil file, and putting soil initial condition in the FileX.

Daily weather data set during the period of field experiment was provided by Prachin Buri Meteorology Station, which located at $14^{\circ} 3' \text{ N}$ and $101^{\circ} 22' \text{ E}$. Precipitation data was collected by the Royal Private Development Project which was

installed at field experimental site. Observed weather data set consisted of precipitation, maximum and minimum temperature. Solar radiation was calculated by using minimum and maximum temperature.

3.5.3 Genetic Coefficients estimation

Genetic Coefficients (GCs) of three flooded rice varieties were estimated by using two GC calculator modules in the DSSAT v4.5, Genetic Coefficient Calculator (GENCALC) and Generalized Likelihood Uncertainty Estimation (GLUE).

GENCALC calculation for genetic coefficients of three rice varieties started with a set of given cultivar coefficients. The model was defined by the user to calculate step-by-step for each coefficient. Beginning with P1 coefficient, which control anthesis date (ADAP: Anthesis Day After Planting), the GENCALC searched for the output file from the crop model and, based on the different between simulated and actual target shown as RMSE (Wallach and Goffinet, 1987). The coefficient could be increased or decreased for optimization to minimize the RMSE between observed and simulated values. The new coefficient could be inserted into rice genetic cultivar file both automatic and manually. Then calculation was repeated by using the new inserted coefficients until it was satisfied for minimum RMSE and RMSEn (Wallach and Goffinet, 1987; Loague and Green, 1993). The same procedure was repeated for calculation of P2O, P2R, P5 G1, G2 and G3 coefficient, respectively (Figure 8).

The GLUE program was written by Paul Wilkens (He *et al.*, 2008) as an integral tool of the DSSAT v4.5 package. It could be accessed from the DSSAT tool menu to start the procedure (He *et al.*, 2008; 2010). The user could select a crop and

cultivar for calculation coefficients. After selecting “Go” button on the screen, the list of list of experiment and treatments was shown up. Experiment and treatments were selected to simulate using the Monte Carlo method to estimate the coefficients that give the maximum likelihood for both growth and phenology observation values (He *et al.*, 2008). Among eight genetic coefficients of rice cultivar, changing of G4 coefficient was able to affect on other coefficients. Other coefficients could be changed by the change of G4 coefficient during running GLUE program. Prior to run GLUE program, the G4 coefficient needed to be manual calibrated (with no range for random) and reran for the most proper value of one variety (The G4 in this research was 1.25) before setting GLUE program to run for all parameters of each variety. The GLUE GC result was searched by selecting the “View Cultivar Coefficient” and copied into the CUL file for further simulation (Figure 9).

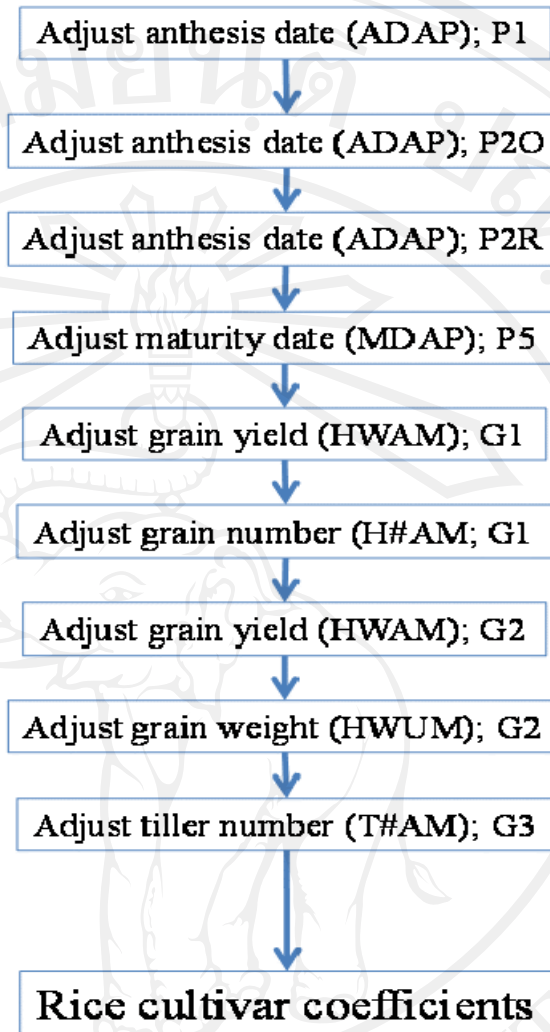


Figure 8 The sequence of optimizations for calibrating the cultivar coefficients using GENCALC

3.5.4 Model evaluation

The calibrated GC of three rice varieties from the two GC estimators were used to run the CSM-CERES-Rice model for simulation of rice development, growth, and yield under different planting date of flooded rice production in deepwater area.

Growth, development, yield and crop N uptake values of simulation and observation were compared.

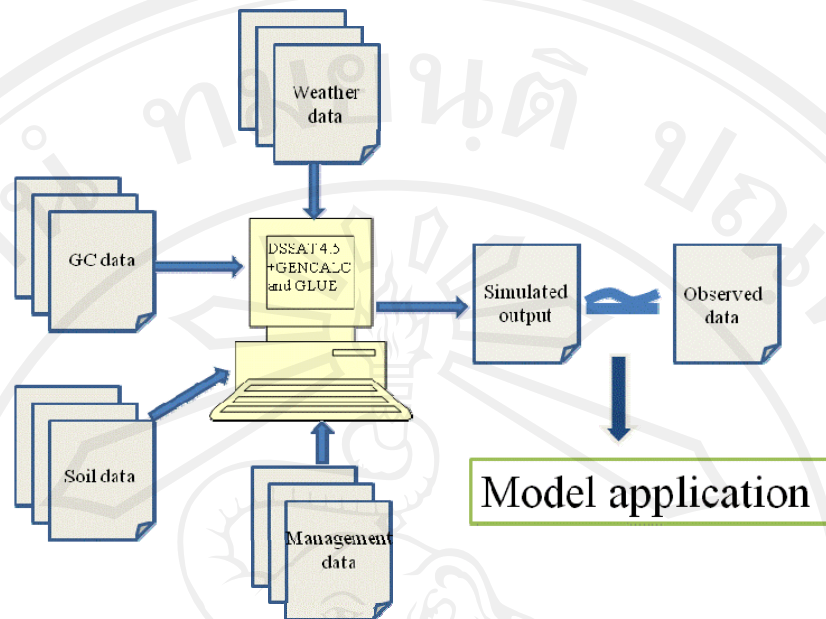


Figure 9 Input data sets and outputs of CSM-CERES-Rice simulation (DSSAT v4.5)

3.5.5 Data analysis

Integration of statistic analysis techniques were used for calculation that included arithmetic mean, standard deviation and analysis of variance (ANOVA) for treatment means comparison. Partial Factor Productivity (PFP) from applied nitrogen fertilizer was also calculated to evaluate efficiency of the fertilizer used for the FDR production in the DWR area.

Farmers concerned with the profit and the returns from increase of investment in the input like chemical fertilizer. The incremental efficiency or agricultural efficiency (AE) and the Partial Factor Productivity (PFP) from applied nitrogen fertilizer were calculated to evaluate efficiency of fertilizer used of flooded rice production in deepwater rice as the following equations (Cassman *et al.*, 1998).

$$AE = \frac{\Delta Y}{N_p} \quad (1)$$

$$PFP = \frac{Y_p}{N_r} + AE \quad (2)$$

where: AE : the incremental efficiency or Agricultural Efficiency from purchase N input

PFP: Partial Factor Productivity

ΔY : the incremental increase in grain yield that results from N application.

Y_o : grain yield without N input

N_r : nitrogen rate applied

Calculation used in this research were RMSE (Root Mean Square Error), RMSEn (Normalized Root Mean Square Error), SD (Standard Deviation), R^2 (R square), and D-index or d-Statistics (index of agreement).

The RMSE was used to compare the difference between observed data from field experiment and simulated data from crop simulation model. The model reproduced experimental data perfectly when RMSE value was 0 using the following formula:

$$RMSE = \left[N^{-1} \sum_{i=1}^N (p_i - o_i)^2 \right]^{0.5} \quad (3)$$

where: p_i : simulated value

o_i : observed value

N : number of observation (equal to number of simulation)

(Wallach and Goffinet, 1987; Timsina and Humphreys, 2006)

The RMSEn was computed for each parameter to compare the outputs from simulation against observation data using the following equation;

$$RMSEn = \frac{RMSE \times 100}{\bar{o}} \quad (4)$$

where: \bar{o} : the overall mean of observation values

(Loague and Green, 1993)

The D-index or d-statistic was a descriptive (both relative and bounded) measure, it was applied to calculate the agreement between observed values and simulated values. It ranged between zero to one, with one being the best fit (Timsina and Humphreys, 2006; Anothai, *et al.*, 2008). The formula to calculate the D-index was shown below:

$$D - index = 1 - \left[\frac{\sum_{i=1}^n (p_i - o_i)^2}{\sum_{i=1}^n (|p_i'| + |o_i'|)^2} \right] \quad (5)$$

where: p_i' : $p_i - \bar{o}$

o_i' : $o_i - \bar{o}$

R^2 value ran from 0 (proposed model does not fit at all) to 1 (proposed model fits the data perfectly). The calculation was as follows:

$$R^2 = 1 - \frac{\sum_i (y_i - y_i^p)^2}{\sum_i (y_i - \bar{y})^2} \quad (6)$$

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad (7)$$

where: y_i : observed i^{th} of parameter y

y_i^s : simulated i^{th} of parameter y

\bar{y} : arithmetic mean of parameter y

n : number of parameter y

(Kammen and Hassenzahl, 2001)