

# Revised fertilizer distribution for CAPRI

## Stable Release 2

Torbjörn Jansson

Swedish University of Agricultural Sciences and AgriFood Economics Centre

[torbjorn.jansson@slu.se](mailto:torbjorn.jansson@slu.se)

Box 7013, SE-750 07 Uppsala

+46-18-671788

## CONTENTS

Acknowledgement .....	1
Summary .....	2
Revising the fertilizer distribution in CAPRI .....	2
The key problem with the fertilizer distribution .....	2
Overview of methodological modifications.....	3
Nutrient balance equations in the simulation model.....	3
A new bi-level programming model of nutrient flows.....	6
Parameterizing the gamma densities.....	7
Numerical considerations.....	8
New data needs .....	10
Integration into the CAPRI system .....	11
Regional time series.....	11
Base year.....	12
Baseline calibration.....	13
Simulation.....	14
Stability tests.....	14
Open issues .....	15
Appendix 1: Completing the square.....	17
Appendix 2: Stability of all fertilizer calibration results.....	18

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## SUMMARY

One specific task of this Stable Release project for CAPRI is to revise the fertilizer module of CAPRI in order to make it more stable. To that end, we proposed and implemented a Bayesian device in the *simulation engine* that chooses the fertilizer distribution that maximizes a joint posterior density function for fertilizer flows. The intuition is that flows in simulation are likely to be “similar to” flows in a reference point (calibration). The economic interpretation is that the decision of how to allocate fertilizers is separable from the decision of what to produce, i.e. the producer can first choose about the cropping plan, merely making sure that a feasible solution to the fertilizer distribution problem exists, and afterwards choose precisely how to satisfy the fertilization needs.

Intimately linked to the Bayesian device in the simulation engine is a corresponding Bayesian estimation that is utilized in the calibration of fertilizer flows, based on exogenous priors for fertilization activities. The code is minimally restructured, which implies using the same crop nutrient balances as before, and maintaining the iterative solution in calibration that goes from higher to lower geographical levels. As the stability experiments reveal, the new system has the potential to do away with numerical instabilities caused by the fertilizer system under repeated starts with a recent GAMS distribution (24.9), but still returns somewhat different results if an older GAMS version (24.7) is used.

An associated task was to aid in the revision of the fertilizer distribution module of IFM-CAP. Since this task is largely isolated from the work in CAPRI, it is reported in a separate deliverable D4b.

## REVISING THE FERTILIZER DISTRIBUTION IN CAPRI

### The key problem with the fertilizer distribution

In STAR 1, it was found that the fertilizer distribution to crops was not numerically stable under repeated experiments. In particular, it became obvious for the calibration step. In contrast, in the simulation step, there was (and still is) a mechanism in place that does not report the actual fertilizer allocation, but merely scales the calibrated allocation so that it fits the simulation result, and hence any instability is hidden.

Analyses of the model performance and code indicated that the primary cause of the instability was an *indeterminacy* in the model structure: There were many possible solutions to the fertilization problem (fertilization plans) that all used the same total quantity of each fertilizer source and satisfied the same total need per crop, and that were all leading to the same level of profits for the representative farm. Furthermore, all linear combinations of such equivalent fertilization plans were also equal from the perspective of the decision maker.

The indeterminacy was present both in the calibration step and the simulation step. In the calibration step, it was playing out most strongly in potassium and phosphorous, where there were fewer priors used. Even though the instability was irrelevant from a production economic and market point of view, it was problematic from a biophysical perspective. In particular, it would lead to different GHG emission coefficients per kg of product, and could also lead to different nutrient surplus per crop, which is problematic for the downscaling to HSMU.

In addition to the indeterminacy, there was also a suspicion of numerical instabilities due to the way the calibration problem was formulated, so that not always a true optimum was found in the estimation nutrient flows. The problem was possibly badly scaled in parts. Because of the dominance of the first problem (the indeterminacy), it was difficult to analyse the possible numerical instability due to scaling, and it was decided to postpone the analysis of scaling and other numerical issues until the indeterminacy had been resolved.

## **Overview of methodological modifications**

The strategy followed in this revision is to make minimal changes to the biophysical foundations of the fertilization system, while resolving the indeterminacy in fertilizer flows. That is achieved by maintaining the economic optimization problem of the regional representative farm, and adding a separate problem for the fertilizer allocation. This means that the optimization of production does not depend on the allocation of fertilizer sources, but only on a weaker condition of “sufficient nutrients being present in the system”. Then, in a second level of optimization, the various nutrient sources are allocated across crops in a way that is as “similar as possible” to a reference situation. This turns the model into a bilevel optimization one, where the upper level is the familiar regional farm optimization model of CAPRI, where the lower level is a statistical model minimizing deviations from a prior distribution, taking the solution from the farm optimization as given.

The only modification that was needed of the regional farm optimization model was to remove the minimum constraint on mineral nitrogen per crop during simulation (but not during calibration). The constraint, which was rarely used, was removed because it would introduce a bound in the lower level model (allocation to crops) that would lead to *complementary slackness conditions* and numerical difficulties. Whether alternative formulations with similar effect as a lower bound on Nitrogen application could be re-introduced needs to be analysed.

In order for the lower level problem to be a true sub-problem (separable) to the farm optimization, it is implemented in terms of its optimality conditions. To avoid the optimality conditions having complementary slackness condition (which would be numerically difficult to solve as constraints to another model), we choose a density function for the inner model that goes to zero when a flow goes to zero, while having an infinite upper bound. The GAMMA density function has that property (support from zero to infinity), while being numerically straightforward to implement (depending on the logarithm function and two parameters).

The parameters of the GAMMA density are calculated during the calibration step by solving the same highest posterior density function as in previous CAPRI models, but now augmented with a gamma distributed prior for fertilizer allocations. When the parameters of the gamma function have been computed, they are stored and used in subsequent simulations.

## **Nutrient balance equations in the simulation model**

We distinguish the three macro-nutrients N, P and K. The supply and uptake of those nutrients are modelled in a uniform way, save for the fact that there is fixation and atmospheric deposition only of N.

Each crop has a requirement per hectare, calculated based on the yield. Yields are exogenous from the vantage point of the producer, but there are alternative technologies available for each cropping activity, and a separable, i.e. handled outside of the optimization model, relation between prices and optimal yields.

From the basic nutrient requirement we first deduct the rate of biological fixation (only for nitrogen and selected crops). The remainder is inflated by a (calibrated) factor and additive term of over-fertilization, and then scaled with a soil-specific factor (only for nitrogen), to arrive at the total amount of nutrients that need to be supplied to the crop. This is the left hand side of Equation 1.

Nutrient supply, shown on the right hand side of Equation 1, comes from mineral fertilizer, manure, crop residues and atmospheric deposition. Mineral fertilizer may have ammonia losses during application. For manure, there are both losses and inefficiencies. When manure is applied to crops, there is an efficiency factor applied to the nutrient content (denoted by  $\phi_{r,excr,n}$  in Equation 1), corresponding to the Fertilizer Value (FV) of manure relative to mineral fertilizer. The efficiency factor is the key parameter of interest in the simulations that we carry out in this study. Crop residues can be re-distributed among crop groups for annual arable crops but not for grassland and permanent crops, where it stays with the crop that produced it. For Crop residues there is both a loss rate and a fertilizer value.

Equation 1: Fertilization requirement function in CAPRI

$$\begin{aligned} & \sum_{i \in I_{j,k}} [levl_{rik} (ret_{rni} (1 - biofix_{rni}) \lambda_{rnik}^{prop} + \lambda_{rni}^{const}) soil_{rn} y_{frik}] \\ & = fmine_{rnj} (1 - loss_{rn}) + fexcr_{rnj} \phi_{r,excr,n} + (1 - isPerm_j) fcres_{rnj} (1 - loss_{rn}) \phi_{r,cres,n} \\ & \quad + isPerm_j \sum_{i \in I_{j,k}} levl_{rik} res_{rni} (resf_{rink} + 1) (1 - loss_{rn}) \phi_{r,cres,n} \\ & \quad \forall r, j, n \end{aligned}$$

Indices in Equation 1:

$r$	region
$i$	crop
$j$	crop group
$k$	technological crop option (high/low yield)
$n$	nutrient (N, P, K)
$isPerm_j$	indicates that crop group $j$ contains permanent crops

Endogenous choice variables in Equation 1:

$levl_{rik}$	Area (ha) of each crop $i$ and technology $k$ in region $r$ .
$fmine_{rnj}$	Application of mineral fertilizer $n$ to crop group $j$ in region $r$
$fexcr_{rnj}$	Application of manure $n$ to crop group $j$ in region $r$
$fcres_{rnj}$	Allocation of crop residue $n$ to crop group $j$ in region $r$ .

Parameters in Equation 1:

$ret_{rni}$	Retention (uptake) of nutrients by the crop
$res_{rni}$	Crop residues output
$resf_{rink}$	Deviation of crop residues output of technology $k$ from mean
$biofix_{rni}$	Biological fixation, share (only for N and selected crops)
$\lambda_{rnik}^{prop}$	Over-fertilization factor, calibrated
$\lambda_{rni}^{const}$	Over-fertilization term, calibrated
$soil_{rn}$	Soil factor
$yf_{rnik}$	Yield factor for technologies
$loss_{rn}$	Loss rate
$\phi_{r,excr,n}$	Nutrient availability ratio for manure
$\phi_{r,cres,n}$	Nutrient availability ratio for crop residues

The reader may have noted that there is no loss rate for manure in Equation 1. CAPRI does contain such loss rates, but they are specific for each animal type and therefore happens on the manure supply side of the regional manure balance (see Equation 2).

The model contains three types of manure: N-manure, P-manure and K-manure. From an agricultural point of view this may seem odd. It might be more intuitive to think of one type of manure per animal category. The motivation is to keep the system simple and flexible. With the present representation, where each animal category supplies N, P, and K-manure, the number of manure classes can be limited and yet the unique mix of nutrients from each animal category can be defined.

The supply of each manure type is collected in a “pool” for each regional farm model, i.e. for each NUTS2-region. Regions within a member state may trade manure, subject to a cost. The supply in the pool plus the traded quantities has to be distributed to the crops in the region, i.e. there is an equality-restriction in place.

Equation 2. Regional manure nutrient balance

$$\sum_j f_{excr_{rnj}} + \sum_s T_{rs} nutshr_{rn} = \sum_{i \in isAnim_{i,k}} lev_{rik} o_{rnik} (1 - loss_{rin}) \quad \forall r, n$$

Where

$o_{rnik}$  is the output of manure nutrient  $n$  from animal type  $i$  using technology  $k$  in region  $r$ ,  
 $nutshr_{rn}$  is the average content of each nutrient in the regional manure pool,  
 $T_{rs}$  is the quantity of manure traded from  $r$  to  $s$ ,  
 $isAnim_i$  indicates that activity  $i$  is an animal production activity

Equation 3: Crop residues balance

$$\sum_j f_{cres_{rnj}} = \sum_{i \notin isPerm_{i,k}} lev_{rik} res_{rni} (techf_{rink} + 1)$$

Where

$isPerm_i$  Is an indicator function defining if crop  $i$  is a permanent crop

Equation 4: Mineral fertilizer balance

$$\sum_j f_{mine_{rjn}} = -netPutQuant_{rn}$$

Where

$netPutQuant_{rn}$

is the net sales (sign convention) of mineral fertilizer

### **A new bi-level programming model of nutrient flows**

One flow from a source  $s = \{\text{mine, cres, excr}\}$  to a sink  $j = \{\text{crop groups}\}$  can in general be anything from zero and upwards. The nutrient balance equations above do not uniquely determine each flow of nutrients from sources to sinks, but it is indeed possible that in one simulation, say, a particular crop group gets much crop residues and little manure, whereas the opposite holds in the next simulation. The total balances will hold equally well in either situation, and the profits will not be affected since the same total amount of mineral fertilizer is purchased, but we do have a stability problem for the model. Furthermore, the different nutrient flows may influence the greenhouse gas emission coefficients of crops (if e.g. the emissions of enteric fermentation follows the manure to the crops). The problem is under-determined, or ill-posed.

To resolve the ill-posedness of the fertilizer distribution, we propose a probabilistic approach. This means that we do *not* introduce any additional economic model for the allocation that somehow makes increasing fertilizer flows more expensive. Instead, we assume that whatever the reasons the farmers have for choosing a particular distribution, those reasons are similar in two simulations, and therefore the fertilizer flows are also similar. Thus, a larger deviation from some reference flows is deemed improbable, albeit not costlier than the situation with the reference flows.

To develop this probabilistic model, we assume that the decisions of the farmer are separable and taken in two steps: first, the farmer decides about the cropping plan and just ensures that the total amount of fertilizer available is sufficient. This is called the *outer model*. Then, a statistical model is solved that finds the most probable fertilizer flows out of the continuum of possible ones. This is called the *inner model*. The structure with outer and inner models makes the problem a bi-level programming one.

To implement the bi-level programming problem in a way that does not change the present structure of the model (with just one optimization solve of the representative farm model) we implement the inner model by its optimality conditions. By carefully choosing the proper probability density functions we ensure that no complementary slackness conditions are needed, so that the inner model is simple to solve. For this the *gamma density* function is very suitable, as it has a support from zero to infinity, with a probability that goes towards zero as the random variable goes to zero.

The parameters of the gamma function are determined in the calibration step, described further below, and then kept constant in simulation. The gamma density function for some random variable  $x$  has the form

$$p(x|\alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}$$

where  $\Gamma(\alpha)$  is the *gamma function*, and  $\alpha$  and  $\beta$  are parameters that determine the shape of the density function. The gamma density is nonlinear, and the joint density, being the product of the densities of all nutrient flows, is even more so. In order to reduce nonlinearity we note that are interested in finding the *highest posterior density*, i.e. maximizing a joint density function, and since the maximum is invariant to monotonous positive transformations we compute the logarithm of the joint density, which will be the sum of terms like the following (the constant term has been omitted since it also does not influence the optimal solution for  $x$ ):

$$\log p(x|\alpha, \beta) \propto (\alpha - 1) \log x - \beta x$$

In our application,  $x$  will be the nutrient flows from sources to sinks. As those can be vastly different for different regions, crops and nutrients, there are likely to be scaling issues when the same equation contains terms with vastly different variable levels and derivatives. To avoid such scaling problems, we note that we can normalize all the gamma densities to have the same mode, for instance “1”. Thus, we can choose as our random variables not the flows directly, but the flows divided by their prior modes (denoted by a “ $\widehat{hat}$ ”):

$$\begin{aligned} x_{rn,excr,j} &= \frac{f_{excr_{rnj}}}{\widehat{f_{excr_{rnj}}}} \\ x_{rn,cres,j} &= \frac{f_{cres_{rnj}}}{\widehat{f_{cres_{rnj}}}} \\ x_{rn,mine,j} &= \frac{f_{mine_{rnj}}}{\widehat{f_{mine_{rnj}}}} \end{aligned}$$

With the normalization above, each density function has the mode of “1”.

During the development process of this revision, many different versions of the scaling was developed, and when this report was written, the current version of the code implemented the scaled density functions in the primal estimation model for fertilizer flows, but the unscaled version in the supply models (i.e. not using normalized random variables but the flows in tons). The reason for using different version is that the algorithms used by the solver software faces different problems when working with the primal (optimization) or dual (solving an equation system).

Assuming that we somehow obtain a prior mode, we need yet another piece of information to determine the two parameters of the density functions. We choose to define the standard deviation of  $x$  in relation to the mode – a ratio that we call “accuracy” – and which indirectly defines the variance. Formally, “accuracy”  $k = \mu/\sigma$ . We get back to the empirical specification of that “accuracy” ratio later.

## Parameterizing the gamma densities

Translating our priors on “mode” and “accuracy” to  $\alpha$  and  $\beta$  involves solving the following quadratic equation system for positive roots:

$$\text{accuracy} = k = \frac{\mu}{\sigma}$$

$$\begin{aligned}\text{mode} &= \mu = \frac{\alpha - 1}{\beta} \\ \text{variance} &= \sigma^2 = \frac{\alpha}{\beta^2}\end{aligned}$$

The first equation is our own definition. The second and third follow from the definition of the gamma density functions. The “accuracy” and “mode” are given. Solving the accuracy definition for  $\sigma$  and the second for  $\alpha$  and inserting into the last equation gives us a quadratic equation in  $\beta$ . Completing the square and discarding the negative root gives us the solution, and this procedure is described in detail in appendix 1. Thus, the log density function is (up to an integrating constant) equal for all nutrient flows:

$$\beta = \frac{\mu}{2\sigma^2} + \sqrt{\frac{\mu^2 + 4\sigma^2}{4\sigma^4}} = \frac{1}{2\sigma^2} (\mu + \sqrt{\mu^2 + 4\sigma^2})$$

$$\alpha = \sigma^2 \beta^2$$

For our normalized fertilization flows,  $\mu = 1$ , we denote the corresponding parameters by a tilde “ $\sim$ ”. The expression for  $\tilde{\beta}$  becomes

$$\tilde{\beta} = \frac{1}{2\sigma^2} (1 + \sqrt{1 + 4\sigma^2})$$

Furthermore, we may define  $\sigma$  in terms of mode as  $\sigma = \frac{\mu}{k}$  where  $k$  is the positive real number that we call “accuracy”. Then, an alternative expression for the alpha and beta parameters of the normalized version  $\tilde{\alpha}$  and  $\tilde{\beta}$  becomes

$$\tilde{\beta} = \frac{k^2}{2} \left( 1 + \sqrt{1 + \frac{4}{k^2}} \right), \quad \tilde{\alpha} = \frac{\tilde{\beta}^2}{k^2}$$

The problem to maximize the joint probability, subject to the constraints that the source-equations and nutrient needs balance. That means solving the following system:

$$\max \sum_{rnsj} \left( (\tilde{\alpha} - 1) \log x_{rnsj} - \tilde{\beta} x_{rnsj} \right)$$

subject to

$$\begin{aligned}x_{rn,\text{excr},j} &= \frac{f_{\text{excr}_{rnj}}}{\widehat{f_{\text{excr}_{rnj}}}} \\ x_{rn,\text{cres},j} &= \frac{f_{\text{cres}_{rnj}}}{\widehat{f_{\text{cres}_{rnj}}}} \\ x_{rn,\text{mine},j} &= \frac{f_{\text{mine}_{rnj}}}{\widehat{f_{\text{mine}_{rnj}}}}\end{aligned}$$

and equations 1, 2, 3 and 4.

## Numerical considerations

Trials with the applied system suggested that albeit the normalization is an advantage in the primal optimization, i.e. in the calibration of fertilizer flows, the same is not true for



the inner model in simulation. With the normalized version, there were frequent tiny infeasibilities turning up in the NUTNED\_ equation, i.e. equation 1 above. The reason for this could not be pinpointed, but we conjecture that it is because of some unresolved closure problem – the first-order conditions of the inner model being binding at the same overall nutrient turnover as the one implied by the NUTNED\_ equation – and that the use of non-normalized variables improves scaling for the solver in this respect because the first-order conditions are modelled in the same units as NUTNED\_. Infeasibilities (which sensitivity experiments sometimes find when using an “old machine” or “old GAMS version”) typically turn up in region-crop combinations that are very small, such as Fodder Root Crops in Prague, or in several of the Norwegian sub-regions.

To reduce the problems in simulation, the currently reported version implements the following first-order conditions (FOC) of the inner model:

Step 1: the straight-forward application of the Lagrangean method.

$$-w_{rnsj} = 0$$

FOC w.r.t.  $fexcr_{rnj}$

$$\frac{\alpha_{r,excr,nj} - 1}{fexcr_{rnj}} - \beta_{r,excr,nj} - v_{r,excr,n} + \phi_{r,excr,n} u_{rnj} = 0$$

FOC w.r.t.  $fcres_{rnj}$

$$\frac{\alpha_{r,cres,nj} - 1}{fcres_{rnj}} - \beta_{r,cres,nj} - v_{r,cres,n} + (1 - loss_{rn}) \phi_{r,cres,n} u_{rnj} = 0 \quad \forall j \notin isPerm_j$$

FOC w.r.t.  $fmine_{rnj}$

$$\frac{\alpha_{r,mine,nj} - 1}{fmine_{rnj}} - \beta_{r,mine,nj} - v_{r,mine,n} + (1 - loss_{rn}) u_{rnj} = 0$$

where  $v$  is the dual value of the relevant “nutrient source equation” out of eq. 2, 3 or 4, and  $u$  is the dual value of equation 1 (NUTNED\_).

Step 2: The system of FOC contains expressions of the type  $1/fmine$  which is likely to impair performance as the second derivatives are not constant (CONOPT computes second derivatives). Therefore, the first term in each FOC was turned into a new variable  $z$  defined as  $z_{r,excr,nj} fexcr_{r,excr,nj} = \alpha_{r,excr,nj} - 1$ , and similar for each source, which is a quadratic expression.

Several alternative formulations were tested and discarded in the process, but can be recovered from SVN: (a) As a prototype evaluation version, the equations defining the new intermediate variable  $z$  were equipped with a small slack by splitting them into two inequalities (similar for all three sources  $excr$ ,  $cres$  and  $mine$ ):

Equation 5:

$$z_{r,excr,nj} \left( fexcr_{r,excr,nj} + \frac{\widehat{fexcr}_{rnj}}{10000} \right) - (\alpha_{r,excr,nj} - 1) \geq 0$$

Equation 6:

$$z_{r,excr,nj} \left( f_{excr_{r,excr,nj}} - \frac{\widehat{f_{excr_{rnj}}}}{10000} \right) - (\alpha_{r,excr,nj} - 1) \leq 0$$

These equations allow the FOC to be binding for a fertilizer flow that is deviating by  $\frac{1}{10000}$  from the value in NUTNED\_ in either direction. (b) Experiments were also made with a version where the slack itself is a variable, the square of which is being minimized, in order to obtain exact calibration. However, such a formulation led to slowed performance and did not help getting rid of the small infeasibilities in NUTNED\_.

## New data needs

Compared with the previous system, the revised fertilizer calibration model also needs prior information on the amounts of fertilizers stemming from each of the three sources mineral, manure and crop residues used per hectare of each crop in each year in the time series. In this project, we investigated the possibility to extract data on *mineral fertilizer application rates* from the FADN data set, where total physical quantities of fertilizers per farm are available as of 2014. The results of that explorative work are reported in deliverable 4b. In the end, we decided not to use the FADN data for estimating priors. The FADN data was made available very late in the project, and so it was impossible to include in the prototype stage, and when it was available, the data set showed some robustness problems that made it more difficult to use. For instance, the units of measurement appeared to differ across regions (Bulgaria seem to be using a different unit than other regions), many zeros reported for farms with non-zero area (see e.g. figure 1 for the Netherlands in deliverable 4b, and the number of non-zeros for Finland reported table 7 of the same deliverable). The new data is also collected only from 2014 onwards, so that some back-casting exercise would be needed in order to create the priors needed for the regional time series of CAPRI (running from at least 1990 to 2013) which would further dilute the empirical content of the priors.

In order to proceed with the methodological developments, we decided to create an interface in the code where prior distributions for fertilizer allocations per hectare can be inserted, and for the time being populate the positions with simple robust blanket assumptions. When better data or external estimates are available in the future, it should be unproblematic to introduce such estimates into the code. The place in the code is indicated in the section on “Regional time series” below. The simple assumption used was that the prior mode = “total nutrient uptake by the crop divided by three”. That is, we assumed a-priori that a third of the nutrient uptake comes from each of the three sources of fertilizers “mineral”, “manure” and “crop residues”.

In order to avoid this assumption dominating the results, a low prior precision (accuracy) was assumed at 0.5, indicating that the standard deviation is two times the mode. The density family was set to “gamma”, prohibiting negative numbers but imposing no upper bound on the outcomes.

Once the estimation has been completed for the regional time series, the system requires no further data, as the estimates from the time series step are used as priors in subsequent calibrations, as described below.

## Integration into the CAPRI system

The fertilizer system is active in two modes (calibration, simulation) and at four points of the system (regional time series, base year, baseline calibration, simulation). We devote one section to each of the latter four points.

Common to all processes is that the equations steering the inner problem are triggered by the existence of a prior on the “y” position, such as

```
p_priFertDist(runr,"priMode",ngrp,fnut,"y")
```

In that way, only one single condition is required. Various tests are applied to ensure that the prior modes are properly set (i.e. all sources and sinks have flows connected to them, and all flows are connecting non-empty sources and sinks).

To ensure an interior solution to the inner problem, we had to remove the equation `NUTMIN_`, which was ensuring a certain minimal application rate for mineral fertilizers. The equation was only removed in simulations. In the estimations/calibrations of fertilizer flows it is still present as before.

The primal density functions are used for estimating the parameters of the fertilizer system (nutrient availability factors etc.), and they are implemented in the file

```
fert\fert_mod.gms
```

The dual equations (first-order conditions) are only used in simulations with the supply models, and are therefore implemented in the file

```
supply\supply_model.gms
```

### Regional time series

This is the first point where the fertilizer calibration is invoked. Fertilization is independently calibrated for each individual year of the time series. The main file controlling that calibration is:

```
fert/ferttrm_years.gms
```

In that file, a general prior mode is assigned for each potential `fertdist`-flow. The empirical foundation could contain engineering knowledge about good fertilization practices. However, for this project we assumed a flat even distribution of total fertilization needs across sources, which probably leads to slightly upward biased estimates in most cases. The prior was set to total need divided by the number of sources available, not considering any losses.

Figure 1 shows the implementation in the code. There are five statements, all modifying the prior parameter `p_priFertDist`. The first and fourth statements are key. In the first statement, the prior mode `priMode` is set for each subregion `ru`, for each `distpos` (mineral, manure, crop residues), each `fnut` (N, P, K), each `ngrp` (crop groups) and `year`. The right hand side show that this is the sum of nutrient uptake in kg per ha for all crops (`MCACT`)

in the current `ngrp` multiplied with the area in thousand hectares, giving total uptake in tons, divided by three. Then, two statements follow that aggregate the regional assumptions to NUTS1 and MS levels. The fourth statement sets accuracy to 0.5 wherever a prior mode has been set. The final step is to use the file `supply\set_fert_priors.gms` to compute the parameters of the gamma density using the mode and accuracy assigned above.

```

119 *
120 * --- Define fertilizer distribution to groups a-priori (prior for estimation)
121 * Here, engineering data or measurements have to be entered - the current code is a simple start
122 * Total retention by crops (in tons) divided by 3.0, i.e. the number of distPos to estimate {mine, excr, cres}
123 * p_priFertDist(ru,"priMode",distpos,fnut,ngrp,YEARS) $ [sameas(distpos,"excr") or sameas(distpos,"mine")
124 * or (sameas(distpos,"cres") and (not PERM_NGRP(ngrp)))]
125 * = SUM( CACT_TO_NGRP(MCACT,NGRP),
126 * data(RU,MCACT,FNUT,YEARS)*data(RU,MCACT,"lev1",YEARS))
127 * /3;
128 *
129 * --- Aggregate to nuts1 and ms
130 * p_priFertDist(nuts1,"priMode",distpos,fnut,ngrp,YEARS)
131 * = sum(MAP_RR(nuts1,ru), p_priFertDist(ru,"priMode",distpos,fnut,ngrp,YEARS) ) ;
132 *
133 * p_priFertDist("%MSLONG%", "priMode",distpos,fnut,ngrp,YEARS)
134 * = sum(MAP_RR("%MSLONG%",ru), p_priFertDist(ru,"priMode",distpos,fnut,ngrp,YEARS) ) ;
135 *
136 * --- With the weak blanket assumption on prior mode, assume a weak prior, i.e. a low accuracy (large variance)
137 * p_priFertDist(RUNR,"accuracy",distpos,fnut,ngrp,YEARS) $ p_priFertDist(RUNR,"priMode",distpos,fnut,ngrp,YEARS)
138 * = 0.5;
139 *
140 * --- Use the priors to derive gamma parameters to use in current experiment
141 * $$$batinclude "supply\set_fert_priors.gms" runr priMode YEARS

```

Figure 1: Entering the prior mode for fertilizer distributions in the code.

The accuracy of this prior was set to 0.5. Given the rule of thumb that “almost all outcomes fall in the range of +/- three standard deviations from the mean”, this implies a weak prior information that easily allows the outcome to be far off the modal value.

The parameters for the fertilizer distribution for all years (as well as the base year) are stored in time-indexed parameters stored in files with the naming pattern

```
%results_out%\fert\prifertdist_%MS%%BAS%.gms
```

where `%results_out%` is the current result directory, `%MS%` is the country code and `%BAS%` is the base year.

### Base year

In the base year database construction, the fertilizer distribution is calibrated for the three year average (base year), controlled by the file

```
fert/ferttrm_bas.gms
```

There, the prior distribution of fertilizer flows for the base year estimation is set to the weighted average of the posterior modes of the underlying individual years, estimated in “CAPREG time series”. The solution is stored on

```
p_priFertDist(%regions%,"postMode",ngrp,fnut,"y")
```

During the base year computations in CAPRI, the supply models are also *solved*, in the process of calibrating the PMP-terms. The key file controlling the base year PMP calibration is:

```
gams\supply\pmp.gms
```

The supply model needs to know what priors to use for the gamma densities of fertilizer flows in simulation. However, the initialization of the supply models is done in a generic initialization file for both CAPREG and CAPMOD (scenario simulation), and that file is called

```
gams\supply\prep_sim.gms
```

This presents the modeller with a difficulty, since we cannot write e.g. “use base year values” or “use target year values”. Instead, the position to load priors from is sent as a *singleton set* called `fertDistPriorYear`, pointing the initialization routine to the correct element in the code of the `prep_sim.gms` file:

```
$$$binclude "supply\set_fert_priors.gms" %regions% postMode fertDistPriorYear
```

The element of `fertDistPriorYear` is defined in `ferttrm_bas.gms`. A more elegant solution would be desirable.

If the model calibrates perfectly, then the *normalized* `v_fertDist` variables are all 1.0 in the optimal solution. This is also verified after optimization of `m_capmodQ`, and an exception<sup>1</sup> is raised if the deviation is greater than 1/1000. The test is only done for the individual regions, not for MS or NUTS1.

### Baseline calibration

In the baseline calibration, the fertilizer distribution is estimated in a way similar to the base year but steered by the file

```
capmod/def_fert_and_requirements.gms
```

There, the prior parameters for the fertilizer flows are defined based on the *posterior* mode of the base year, modified with land use changes: the fertilization per ha is computed in the base year situation and then multiplied with the areas in the calibration point. Accuracy is set to “1.0”, meaning that standard deviation equals mode. Calibration proceeds as in the base year, and the result is stored on the entry of the selected simulation year:

```
p_priFertDist(runr, "postMode", ngrp, fnut, "%simy%")
```

The results are stored inside a file specific for the country, base year and target year:

```
%results_out%\fert\prifertdist_%MS%%BAS%%SIM%.gms
```

---

<sup>1</sup> This exception is raised and causes error messages when the calibration is done on an old machine (4 core machine, +10 years old, see deliverable on sensitivity experiments) or with an old gams version (24.7), especially in parallel execution.

where, in addition to the syntax of the base year calibration, there is an additional suffix for target year. In previous pre-release versions, all parameters (from time series, base year and target year) were stored in just one single file per country, but that provokes file access problems when several target years are calibrated in parallel.

## Simulation

In simulation, the posterior mode of the baseline calibration is used as the prior for the gamma density of the flows, with an accuracy of “1.0”. The data is loaded, and the important set `fertDistPriorYear` is defined, inside the file:

```
capmod\create_sim_ini_gdx.gms
```

## Stability tests

The revised fertilizer distribution method developed in this paper was implemented in STAR 2.1 maintenance release, and subjected to all the stability tests of the Stable Release. Furthermore, new test were added specifically aimed at analysing the results of the fertilizer distribution. The main conclusions from the implementation are

1. The calibration of the fertilizer flows in CAPREG are very stable, albeit not identical in all experiments. Further analysis suggests that the remaining, smaller instabilities that show up with e.g. older GAMS releases, are at least partly trickle-down effects from instabilities in upstream parts of CAPREG time series (land balance consolidation?).
2. With parallel execution of the task “baseline calibration of supply models”, there is risk of a failure of calibration of fertilizer flows when an old machine or older GAMS version is used. A manual restart of the problematic countries generally solved such problems.
3. Despite (2.), the implementation in the STAR was deemed worthwhile, since the stability improvements for model results were vast.

It is not straightforward to compare the stability of the fertilizer allocation relative to the old system, because in previous versions of CAPRI, the fertilizer distribution variables were discarded and the parameters relating to over-fertilization and nutrient availability were stored as indexed dimensions of larger data cubes. And for the results of the general data cube of CAPRI (data) there are many other changes that disturb the picture. Here we make two analyses to support the conclusions above:

Firstly, the stability of the general DATA parameter from CAPREG time series seems to have deteriorated, but that is not due to the fertilizer allocation. By the example of Belgium, we find a very large share of unstable values (measured at machine precision) in the data cube (>90%) when an old GAMS version is used, compared to zero differences for repeated restarts on the same machine with the same software. Digging into the details indicates that entire years and crops are deviating slightly in areas and yields, which of course influences fertilizer allocation.

Secondly, we can now for the first time analyse the stability of each of the estimated parameters steering the fertilizer distribution: the additive and multiplicative over-fertilization factors, the nutrient availability factors for manure and crop residues, and the parameters of the gamma density. A summary of all those estimates of all countries in all years in CAPREG time series and base year are shown in Table 1. Of the 22 million parameters compared, less than 1% differed by more than machine precision,

and a diminutive fraction (7.41E-3 percent of the total) differed by more than one promille. Only 46 numbers out of 22 million differ by more than 10%, and just five numbers appear/disappear compared to the reference experiment.

**Table 1. Summary of stability test of fertilizer calibration in CAPREG. Number of differences in each size class of all the five GAMS parameters generated in the fertilizer calibration.**

<b>Class</b>	<b>Count</b>	<b>Share of total</b>
<b>&gt;zero</b>	215592	0.009852
<b>&gt;0.001</b>	1622	7.41E-05
<b>&gt;0.01</b>	292	1.33E-05
<b>&gt;0.1</b>	46	2.1E-06
<b>&gt;1</b>	6	2.74E-07
<b>&gt;10</b>	5	2.28E-07
<b>&gt;100</b>	5	2.28E-07
<b>infinite</b>	5	2.28E-07
<b>Total</b>	<b>21882237</b>	

## Open issues

The system implemented above appears to be very promising because of two characteristics:

1. It imposes an interior solution for the fertilizer flows and promises stability of the model in that respect
2. It stabilizes the fertilizer flows without influencing how the farm agent in the supply model chooses activity levels – the mechanism is purely statistical, implying no additional economic incentives for the producers. It is therefore “modular”.

The present release demonstrates the feasibility of the approach, and should be mature for applications. The system functioned with all settings tested in the stability experiments carried out. In the process of developments, some features and shortcomings of the system were detected which it would be desirable to address in the future. They are listed here for the purpose of documentation.

- i. The empirical foundation in the estimation of the fertilizer flows is weak. The initial plan was to use FADN data on fertilizer allocation, but that data was deemed insufficient (see section on new data needs above) at the present point in time. Not immediately relating to the present revision, scrutiny of the outputs also suggested that the estimation would benefit from exogenous estimates or revisions of the nutrient availability factors ( $\phi$  in Equation 1) which sometimes come out surprisingly high.
- ii. The hierarchical estimation over MS-NUTS1-NUTS2-FARMTYPE in `m_fertdist` is in-transparent and likely error prone with the iterative error bound opening routine. Re-writing the estimation in a way that no bound-opening is needed in order to be able to analyse performance of the estimator more easily.

- iii. Furthermore, we suspect, but cannot prove, that the estimation does not produce reliable outputs because of scaling issues. This manifests as very large differences in size of the partial derivatives of the objective function of the estimator as computed by the solver routine CONOPT in the program listing file. Experience from optimization with CONOPT in general has shown that such great variability in partial derivatives can be connected with failure to identify the local optimum correctly.
- iv. The `v_fertdist` variables should be reported without modification to the GUI to make it easier to analyse results and understand the mechanics of the model. The present version of the model instead reports a scaled version of the base year fertilizer balances, effectively discarding the output of the fertilizer model.
- v. The NUTNED\_ equation should be disaggregated and reported too. It would be helpful to use the equation itself to find out how left hand side (uptake) and right hand side (nutrient supply) decompose into different components, so that the reports on nutrient balances are directly linked with the supply model equations. A draft on how that could be done was produced jointly by A. Leip, P. Witzke and T. Jansson in the current project, but the work is not supported in any ongoing project and therefore standing still. Such a development would have to take care not to compromise computations of e.g. environmental indicators.

Further down the road, we might investigate the possibility of bringing the fertilizing activities (`v_fertDist`) in line with the DATA accounting principles applied elsewhere, requiring the introduction of more sets for input/output of various nutrients (N, P, K) from various sources (manure, mineral, crop residues) in a generic set driven manner (c.f. `icam/yam` for animals, or `gras/fgra` for feed) paving the way for extension to other balances (carbon?). The equations could be aligned with the farm balance (`supbal_`) system that is used for all other inputs and outputs in a way similar to young animals. This paves the way for a future manure trade module. The reporting to the DATA cube is made to reflect the input/output of all of these new items based on the variables in the optimization model as for all other activities/netsales. With explicit fertilizer activities, it would also be possible to implement alternative fertilization technologies for the farmers to choose among endogenously, in e.g. the mitigation module.



## APPENDIX 1: COMPLETING THE SQUARE

$$\begin{aligned}\text{mode} = \mu &= \frac{\alpha - 1}{\beta} \\ \text{variance} = \sigma^2 &= \frac{\alpha}{\beta^2} \\ \alpha &= \beta\mu + 1 \\ \sigma^2\beta^2 &= \beta\mu + 1 \\ \beta^2 - \frac{\beta\mu}{\sigma^2} - \frac{1}{\sigma^2} &= 0\end{aligned}$$

Subtract the constant from both sides

$$\beta^2 - \frac{\beta\mu}{\sigma^2} = \frac{1}{\sigma^2}$$

Add the square of half the linear coefficient  $\left(\frac{\mu}{2\sigma^2}\right)^2$  to both sides

$$\beta^2 - \frac{\beta\mu}{\sigma^2} + \left(\frac{\mu}{2\sigma^2}\right)^2 = \left(\frac{\mu}{2\sigma^2}\right)^2 + \frac{1}{\sigma^2}$$

Express left hand side as a square and re-arranging the right hand side gives

$$\left(\beta - \frac{\mu}{2\sigma^2}\right)^2 = \left(\frac{\mu}{2\sigma^2}\right)^2 + \frac{1}{\sigma^2} = \frac{\mu^2}{4\sigma^4} + \frac{4\sigma^2}{4\sigma^4} = \frac{\mu^2 + 4\sigma^2}{4\sigma^4}$$

Solving for the positive root gives

$$\begin{aligned}\beta &= \frac{\mu}{2\sigma^2} + \sqrt{\frac{\mu^2 + 4\sigma^2}{4\sigma^4}} = \frac{1}{2\sigma^2}(\mu + \sqrt{\mu^2 + 4\sigma^2}) \\ \alpha &= \sigma^2\beta^2\end{aligned}$$























