# Supplementary material for "RELCA: A REgional Life Cycle inventory for Assessing bioenergy systems within a region"

**S.O.Keeffe[1], S.Wochele-Marx[1], D. Thrän[1,2]**

**1. Helmholtz Centre for Environmental Research (UFZ). Department of Bioenergy. Permoserstraße 15, 04318 Leipzig, Germany**

**2. Deutsches Biomasseforschungszentrum (DBFZ). Bioenergy Systems Department. Torgauer Straße 116, 04347 Leipzig, Germany**

## S1. Example of script to account for regional variation

Below is an example of MATLAB 2012b[i] script used for estimating the nitrogen applied per pixel, based on regionally varying geographical parameters. This was used as part of the example case study presented in the paper. Naturally, the ability to introduce and account for the potential regional variability of fertiliser application, due to the different geographical or spatial characteristics of a particular region (e.g. soils, climate), depends on data availability and available modelling capacity. The output of the CRAMod step should provide a sufficient number of geographical parameters enabling the modelling of such regionally distributed management strategies for each of the constituent grid cells.

*% To estimate the amount of nitrogen fertiliser applied per grid cell ($AppF_N$) the "N-Basis-Sollwert" method (required N rate) was used. This is used as part of best farming practices for the region [1-3], with the recommended N rate dependent on yield, using a modified equation outlined in [1].Crop refers to crop of interest e.g. Rapeseed in this case example. CropNsoll is the base estimation for the amount of nitrogen required.*

Crop.Nsoll (:,1)=0.0268 × Crop.yieldha (:,1) – 1.7143

*% finding where the Ackerzahl number is either greater than 40 or less than 40.*

AzCred1(:,1)=logical(Raps.Az<=40) *% AzCred1= find which grid cells have an Ackerzahl value less than 40*
AzCred2(:,1)= logical(Raps.Az >40) *% AzCred2= find which grid cells have an Ackerzahl value greater than 40*

*% if Ackerzahl is less than 40, an additional 10 kg of fertiliser should be applied to the pixel, if it is greater than 40, than no additional fertiliser required.*

AzCred=Crop.Az;
AzCred(AzCred1,1)=10; % AzCred1= credit for grid cell if Ackerzahl value lower than 40, assign a value of 10
AzCred(AzCred2,1)=0; % AzCred2= no credit for grid cell if Ackerzahl value greater than 40, assign a value of 0
Crop.AzCred=AzCred; % Combining all values into one column

*% to estimate the amount of fertiliser applied – NApplied*

Crop.NApplied(:,1)= Crop.Nsoll (:,1)-(Crop.Nmin(:,1)-Crop.AzCred(:,1));

*% The average mineralized nitrogen in the soil ($CropN_{min}$), estimated for the Böden Klima Region [4] found within CG was used [5], which were derived from various regional reports and datasets [1,6-8,3].*

## S.2 Equations implemented to estimate the potential amount of fertiliser product used in the region.

The background fertiliser product flows should then be determined based on regional statistics if possible. Estimating the amount of fertiliser product required ($FP_i$) per grid cell can also be performed with the relevant programming script, such as MATLAB 2012b[i] shown in the example above.

### *Estimations for fertiliser product applied*

$$F_m = F_i + F_j + .. F_n \qquad (1)$$

$F_m$ = total amount of fertilising nutrient m (e.g. N, P, K) sold in a particular region (e.g. county, federal state) in one year (kg /a)

$F_i$ = amount of fertilising nutrient sold as fertiliser product i (kg /a).

$F_j$ = amount of fertilising nutrient sold as fertiliser product j (kg /a).

$F_n$ = amount of fertilising nutrient sold as nth fertiliser product (kg /a).

$$F_{i,share} = \frac{F_i}{F_m} \qquad (2)$$

$F_{i,\ share}$ = the share of fertilizing nutrient sold as fertilizer product F*i* (kg/kg). This is also applicable for i to the nth fertilizer product.

### *Estimations for fertiliser product applied on a per Grid cell basis*

$$F_{m,fi} = AppF_m \times F_{i,share} \qquad (3)$$

$F_{m,fi}$ = the amount of fertilizing nutrient *m* contributed by the fertilizing product $F_i$ for the fertilizer applied (kg per grid cell).

$AppF_m$ = the amount (kg) of fertilizer m applied in the regional foreground per ha as part of the regional energy crop management.

$$FP_i = \frac{F_{m,fi}}{X_{nut,i}} \qquad (4)$$

$FP_i$ = the amount of fertilizer product required to deliver $F_{m,fi}$ (kg)

$X_{nut}$= the amount of fertilizer nutrient m present in fertilizer product $F_i$ (kg)

## S.3 Overview of data format and aggregation for non- regional flow modelling

***Conventional life cycle calculations (discussion based on [9])***

In general matrix algebra is used to solve life cycle equations, where columns of the matrix in general refer to production processes (e.g. cultivation) and rows refer to flows (e.g. kg fertiliser, yields or MJ of electricity). The general solution equations for life cycle are as follows;

$$s = A^{-1}f \qquad (5)$$

$$g = sB \qquad (6)$$

$$h = Qg \qquad (7)$$

The technology matrix A (containing the coefficients for all activity flows e.g. kg of fertiliser), is assumed to be square (e.g. same number of columns and rows) and therefore, under the rules of matrix mathematics can be inverted to $A^{-1}$. This is then multiplied by the functional unit (f) or demand function vector e.g. 1 MJ of biofuel, in order to find the scaling vector s. The derivation of the s vector essentially determines the fraction coefficient for each input flow in our inverted technology matrix $A^{-1}$, e.g. what fraction of the original flow (which may have been calculated or provided with a differing unit, such as per hectare), is required to meet the designated demand function of e.g. 1 MJ. In other words, how much nitrogen fertiliser is required in the production of 1 MJ of my biofuel (kg fertiliser per MJ)? The *s* vector should have the same number of rows as our environmental interventions matrix B has columns. It is then multiplied with the environmental interventions matrix B (containing all the associated emissions related to the activity flows in technology matrix A), in order to scale the environmental interventions produced in the production of, for example, 1 MJ of biofuel. The solution of the life cycle inventory is the vector g, in which all the burdens are aggregated across the whole supply chain, regardless of where they were produced or released (Hauschild 2006a), e.g. the total amount of $N_2O$ released per MJ of biofuel.

In order to have a clearer understanding of the computational structure of LCA, we also discuss briefly the impact assessment phase, LCIA. The LCIA is the second step in which each environmental burdens in the LCI (i.e. all the rows in g) are multiplied with the characterization factor coefficients in the matrix Q, weighting their contribution towards a particular environmental impact (h). Characterization factors (CF) are usually derived using different physically based models which reflect the general mechanics of emission sources, dispersion, deposition and potential risk of environmental impacts [10]. Characterization factors used for estimating the potential contribution to the different impacts are usually already integrated within commercially available life cycle software and are usually site generic (i.e. no consideration for where the impacts occur)[11]. Thus, the software solves the life cycle balances, providing the list of impacts (h) associated with producing 1 MJ of biofuel.

***RELCA life cycle accounting approach***

When greater spatial details are to be introduced, the matrix algebra outlined above needs to be adapted to account for the locations of the various activities. In other words for every new location, we need to add a new row [12,9]. The additional increases in rows can alter the shape of our technology matrix and make it rectangular (less processes than flows), making the inversion of the matrix A more difficult to implement [13] and therefore, solving for g or h. Several approaches are proposed in the literature to overcome this bottle neck of trying to introduce greater spatial details life cycle approaches focusing on a "within regional context". However, further discussion on this is outside the scope of this paper; please refer to [13-15].

The RELCA approach in its current version (v1.0), used for estimating GHG balances, is rather simple from this perspective and in this first step avoids the need to modify the Life cycle matrix structure or the need to reconfigure the geographically modelled data to fit the life cycle matrix structure (see Figure S1). This is mainly done through the use of bioenergy catchments. In other words, the calculated foreground (inputs flows (M) and emissions (E)) flows are aggregated to a per catchment basis. This is mainly implemented for the regionally distributed biomass production, i.e. all flows relating to biomass production are aggregated per catchment and then divided by the total amount of biomass supplied to the bioenergy plant (e.g. kg rapeseed used). Figure S1 and equation 8, provide an overview of how regionally distributed data is structured and then delineated to a per catchment basis (the delineation is done as part of the CAM step).

In RELCAs current form (i.e. focusing on GHG production), these normalized flows ($M_{n,i}$) for each bioenergy plant catchment are then inputted into the life cycle software in order to; 1) make the connections between the regional foreground and non-regional indirect flows (e.g. linking to upstream processes such as fertiliser production) in order to effectively implement the life cycle matrix accounting for the regional production of a bioenergy product; 2) to estimate the scaling vectors, or the total amount of input required per functional unit measure of the bioenergy system (e.g. MJ produced). The later can then be used to help model and validate the non-regionally induced GHGs on a grid cell basis (eq. 9-10). Technically speaking , converting all emissions to $CO_2$ equivalents is a characterisation step performed in the LCIA phase of LCA, here we use it here to simplify the summation of the LCI, as is common practice in life cycle approaches for estimating GHG emissions. Additionally, as GHGs are classified as regional burdens with global impacts [16] and are site generic [11], the summation of these emissions in a GHG category is permissible in a regional distribution, as there is no need to have a regionally distributed impact assessment.

$$M_{n,i} = \frac{\sum_{m=1}^{x} M_n}{\sum_{m=1}^{x} Y} \quad (8)$$

x= number of grid cells associated with the plant catchment.

$M_{n,i}$ = the summed total amount (kg)of management parameter ($M_n$) required per kg of energy crop supplied to the bioenergy plant *i*.

$M_n$ =the amount of management input required per grid cell.

Y= the yield per grid cell.

The same calculation are also carried out for Emissions ($E_{n,i}$). Both the $M_{n,i}$ and $E_{n,i}$ are then used as input/emissions flows into life cycle inventory software (e.g. GaBi, Open LCA, SimaPro).

For determining the potential GHG balances of a regional bioenergy product, RELCA can also be used to estimate both the direct and induced indirect flows and emissions estimated per functional unit of energy or per hectare supplied for the constituent grid cells. Such calculations are again estimated by means of catchment delineation (9-10). The estimates for the non-regional burdens can be taken from the upstream data bases (e.g. Ecoinvent, GaBi)[i] or form various literature sources. For the GHG emissions, as the non-regional burdens are to be aggregated, it is easier to take the already characterised value e.g. CAN (Calcium ammonium nitrate) fertiliser has an emission factor of 8.69 kg $CO_2$eq/kg [17], see equation 10.

$$M_{n,x,i}\ per\ MJ = \frac{MNR_{n,x}}{E_i} \quad (9)$$

$M_{n,x,i}$ = the amount of Non-Regional management flow n assigned to grid cell x, required per mega joule of bioenergy catchment i output (kg /MJ)

$MNR_{n,x}$ = Non-Regional management flow of product n assigned to grid cell x (kg/grid cell)

$E_i$ = the total energy produced by the associated bioenergy plant i in one operational year (MJ/a) e.g. plant i produces 5,000 tonnes of biodiesel in one year, therefore this equates to approx. $186\times10^6$ MJ (assuming 37.2 MJ/kg biodiesel).

$$MNREmis_{n,x,i} = MNR_{n,x,i} \times EFNR_{n,x} \quad (10)$$

$MNREmis_{n,x,i}$ = the potential GHG emission associated with a particular non-regional management product ($MNR_n$) attributed to the grid cell x in bioenergy catchment i (emissions per ha or grid cell).

$MNR_{n,x,i}$ = Non-Regional management flow of product n assigned to grid cell x (kg or grid cell).

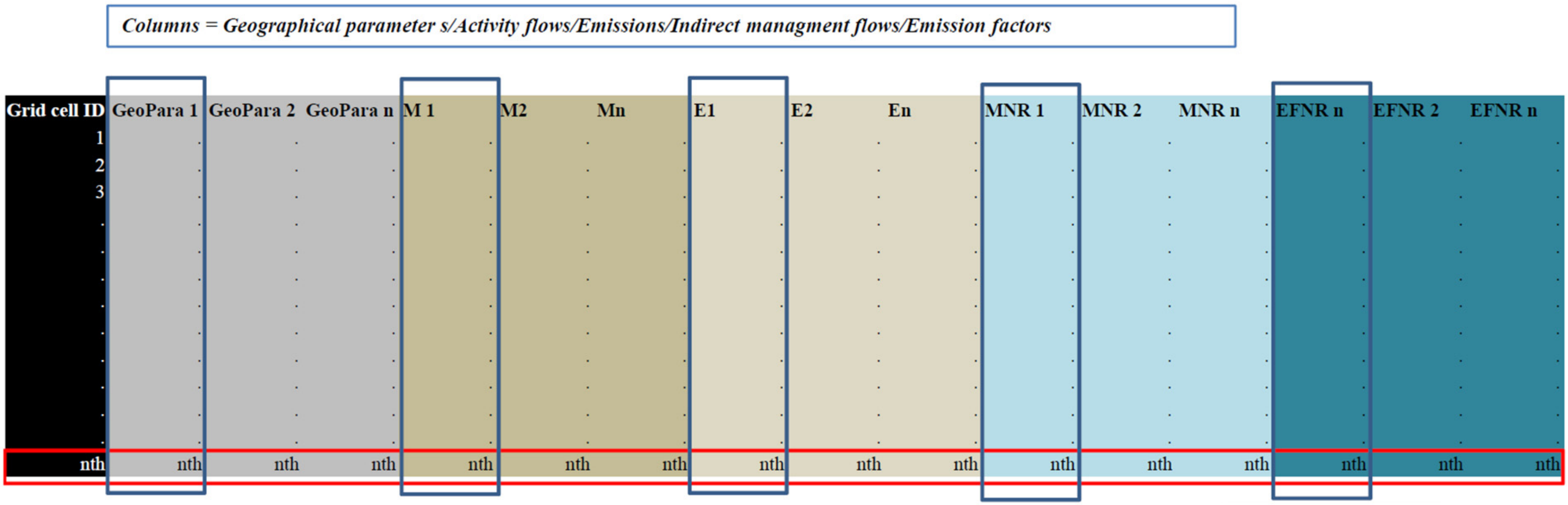
$EFNR_{n,x,i}$= an emission factor for a particular non-regional management product (MNRn) attributed to the grid cell x. These emissions factors can come from literature or from the different databases such as Ecoinvent [18].

For the simple case study presented in this paper, we conducted both approaches, in the life cycle software GaBi 6.0 and in MATLAB 2012b[i] and compared the difference between the estimated GHG emissions for biomass production. The % error between the two are shown in Table S1 below, in general Gabi provided slightly lower estimates than the MATLAB modelling. However, there was very little difference between the two, with most % differences being less than 1%.

Table S1. Percentage (%) difference between life cycle software GaBi 6.0 and in MATLAB 2012b (The Math Works, Inc., Natick, Massachusetts, United States) for estimating the associated cultivation emissions (regional, non-regional).

| Catchments[1] | | | Fertiliser[3] | | | Crop protection[4] | | | Field operations[5] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| No | n | Total [2] | N | P | K | Insecticide | Herbicide | Pesticide | Diesel | Exhaust emissions | Soil emissions[6] |
| 1 | 36 | 0.25 | 0.30 | 0.23 | 0.23 | 0.23 | 0.23 | 0.23 | 0.23 | 0.23 | 0.23 |
| 2 | 70 | 0.51 | 0.40 | 0.56 | 0.56 | 0.56 | 0.57 | 0.56 | 0.56 | 0.56 | 0.56 |
| 3 | 78 | 0.07 | 0.04 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 |
| 4 | 91 | 0.01 | 0.10 | 0.06 | 0.07 | 0.07 | 0.07 | 0.07 | 0.07 | 0.07 | 0.07 |
| 5 | 719 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

1. Catchments No, refers to the catchments of each of the bioenergy catchments presented in the example case study. Catchments n refers to the number of grid cells associated with each catchment.
2. Total refers to the total GHG for cultivation per MJ produced by the catchment (direct regional and induced indirect non-regional).
3. Fertiliser refers to non-regional burdens for production of fertiliser products, nitrogen (N), phosphorus (P) and potassium (K).
4. Crop protection refers to non-regional burdens for production of crop protection products.
5. Field operations refer to non-regional burdens for producing diesel fuel and direct regional burdens relating to the combustion of diesel in the various agricultural machinery, which were used for cultivation e.g. combine harvester.
6. Soil emissions refer here to direct emissions from soil due to nitrogen fertiliser application e.g. $N_2O$.




- GeoPara = Geographical parameters such as soil clay content, Akazahl value etc.
- M1-Mn = Managment flows from 1 to n required for producing biomass on a per ha/grid cell basis e.g. fertilisers, crop protection
- E1-En = Emissions from 1 to n produced as a result of biomass production per ha/grid cell e.g. $CO_2$, $N_2O$, $NH_4$
- MNR1-MNRn = Managment flows which are non -regional e.g. managment products.
- EFRN1- EFNRn= the emission factor associated with producing 1 kg of mangament product MNR1-MNRn

Figure S1. Overview of structure for geographically modelled data.

## S4. Supplementary Material: Example case study

Table S2. Crop management practices identified for the CG region (All units are kg $ha^{-1}$ $a^{-1}$, unless otherwise stated)

| Management | Values kg/ha | Source |
|---|---|---|
| Fertiliser rates | | |
| P [1] | 26-29 | [5,2] |
| K | 29 | [19] |
| Lime | 1000 | [19] |
| Crop protection[2] | | |
| Herbicide [3] | 0.287 | [20-22] |
| Insecticide[4] | 0.072 | [20-22] |
| Pesticide[5] | 0.75 | [20-22] |

1. Phosphorus rates deviated across the associated BKR regions.
2. Amount denotes active ingredients assumed to be applied.
3. Herbicide; (active ingredient=Metazachlor/Clomazone) associated Ecoinvent stream "Cyclic N compound"[23].
4. Insecticide; (active ingredient = Thiacloprid) associated Ecoinvent stream "Diazole compounds"[23].
5. Pesticide; (active ingredient= Tebuconazole) associated Ecoinvent stream "Pesticide Unspecified". [23]

Table S3. Example of Non - regional flows for rapeseed production the percentage contributions of different management products for the region

| Products [1] | SN | SA | Ecoinvent modules[2] |
|---|---|---|---|
| Nitrogen fertilisers | | | |
| CAN | 47 | 41 | RER: calcium ammonium nitrate, as N, at regional storehouse |
| UAN | 19 | 19 | RER: urea ammonium nitrate, as N, at regional storehouse |
| Urea | 12 | 16 | RER: urea ammonium nitrate, as N, at regional storehouse |
| Mix[3] | 22 | 23 | RER: ammonium sulphate, as N, at regional storehouse/ RER: ammonium nitrate, as N, at regional storehouse (50/50 mix) |

1. [24]
2. [25]
3. Mix refers to the combination of ammonium sulphate and ammonium nitrate [24]

**S5. Visualisation of catchment emissions per hectare for the illustrative example.**

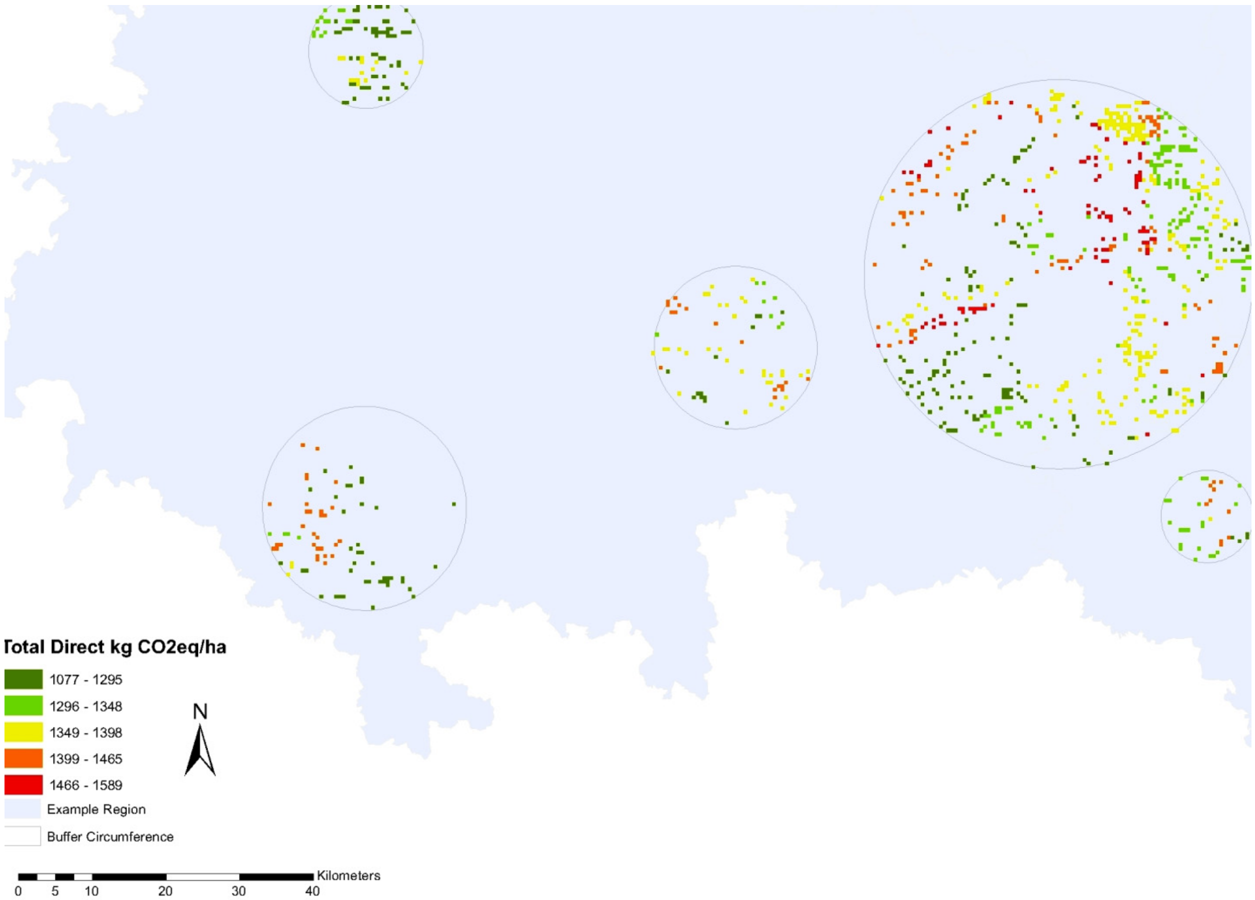



Figure S2. Exemplary map showing the catchment delineated distributions of total direct GHG emissions ($CO_2$eq. $Ha^{-1}$) for rapeseed production within the example region. Map produced using Arc GIS® software by Esri.

For each of the different biodiesel plant catchments a greater spatial variation with regards to emissions per hectare of rapeseed supplied to biodiesel plant can be observed. This is a very important feature of the RELCA output and is an essential component in the interpretation of the final results and how they are potentially influenced across the region due to difference within the regions differing geographical features. The use of the different functional units for visualising and interpreting the RELCA results will be outlined in a succeeding paper (in progress).

## End note

**(i)MATLAB,** The Math Works, Inc., Natick, Massachusetts, United States; PE.**GaBi Software** – Systems and Databases for Life Cycle Engineering. Copy right TM. Stuttgart,Echerdingen 1992-2016; Frischknecht R, et al. (2005) The **Ecoinvent** Database: Overview and Methodological Framework (7 pp). Int J LCA 10 (1):3-9. doi:10.1065/lca2004.10.181.1

## References


1. TLL (2007) Thüringer Ministerium für Landwirtschaft, Forsten, Umwelt und Naturschutz. Landwirtschaft und Landschaftspflege in Thüringen.Düngung in Thüringen 2007 nach "Guter fachlicher Praxis„. Naumburger Str. 98, 07743 Jena

2. LLFG Landesanstalt für Landwirtschaft, Forsten und Gartenbau, Sachsen-Anhalt. Grundlagen der Düngebedarfsermittlung für eine gute fachliche Praxis beim Düngen.

3. BEFU (2013) Düngebedarfsermittlung. Sächsisches Landesamt für Umwelt, Landwirtschaft und Geologie. Available at: http://www.landwirtschaft.sachsen.de/landwirtschaft/1868.htm. Accessed 02.2013.

4. Roßberg D., Michel V, Graf R, Neukampf R Definition von Boden-Klima-Räumen für die Bundesrepublik Deutschland.Nachrichtenbl. Deut. Pflanzenschutzd., 59 (7), S. 155–161, 2007, ISSN 0027-7479. © Eugen Ulmer KG, Stuttgart.

5. Witing F. (Unpublished) Crop Managment Inventory for Central German Region.

6. TLL (2010) Thüringer Ministerium für Landwirtschaft, Forsten, Umwelt und Naturschutz.Aktueller Rat zur Nmin- und Smin-Situation Thüringer Böden im Frühjahr 2010.

7. LLFG (2010) Landesanstalt für Landwirtschaft, Forsten und Gartenbau, Sachsen-Anhalt. Nmin-Vergleichswerte Frühjahr 2010. Available at:http://www.llfg.sachsen-anhalt.de/fileadmin/Bibliothek/Politik_und_Verwaltung/MLU/LLFG/Dokumente/Nmin2010_2.pdf. Accessed 02.2013.

8. LLFG (2010) Landesanstalt für Landwirtschaft, Forsten und Gartenbau, Sachsen-Anhalt. Nmin-Vergleichswerte Frühjahr 2010 – 2. In formation der LLFG Sachsen-Anhalt

9. Heijungs R, Suh S (2002) The computational structure of life cycle assessment. Kluwer Academic Publishers, Dordrecht

10. Bellekom S, Hettelingh JP, Aben J (2009) Spatial aspects affecting acidification factors in European acidification modelling. Environ Modell & Softw 24 (4):463-472. doi:http://dx.doi.org/10.1016/j.envsoft.2008.09.002

11. Potting J, Hauschild M (2005) Background for spatial differentitaion in LCA impact assessment - The EDIP 2003 methodology. Enviornmental Project No. 996, Miløprojekt. Danish Ministry of the Environment

12. Heijungs R (2012) Spatial differentiation, GIS-based regionalization, hyperregionalization, and the boundaries of LCA. In: Ioppolo Ge (ed) Environment and Energy: Editorial series of Italian Commodity Science Academy and Engineering Association of Messina. Franco Angeli, Milano, Italy, p. 165-176

13. Saner D, Vadenbo C, Steubing B, Hellweg S (2014) Regionalized LCA-Based Optimization of Building Energy Supply: Method and Case Study for a Swiss Municipality. Environ Sci Technol 48 (13):7651-7659. doi:10.1021/es500151q

14. Azapagic A, Chalabi Z, Fletcher T, Grundy C, Jones M, Leonardi G, Osammor O, Sharifi V, Swithenbank J, Tiwary A, Vardoulakis S An integrated approach to assessing the environmental and health impacts of pollution in the urban environment: Methodology and a case study. PSEP (0). doi:http://dx.doi.org/10.1016/j.psep.2012.11.004

15. O'Keeffe S, Majer S, Bezama A, Thrän D (Submitted) When considering no man is an Island - assessing bioenergy systems in a regional and LCA context: A review

16. Loiseau E, Roux P, Junqua G, Maurel P, Bellon-Maurel V (2013) Adapting the LCA framework to environmental assessment in land planning. Int J LCA 18 (8):1533-1548. doi:10.1007/s11367-013-0588-y

17. Nemecek T, Erzinger S (2005) Modelling Representative Life Cycle Inventories for Swiss Arable Crops (9 pp). Int J LCA 10 (1):68-76. doi:10.1065/lca2004.09.181.8

18. Jungbluth N, Chudacoff M, Dauriat A, Dinkel F, Doka G, Faist Emmenegger M, Gnansounou E, Kljun N, Schleiss K, Spielmann M (2007) Life cycle inventories of bioenergy. Final report ecoinvent data v2 0 No 17

19. KTBL (2012) Leistungs-Kostenrechnung Pflanzenbau. Available at: http://daten.ktbl.de/dslkrpflanze/postHv.html#Auswahl. Accessed: 11. 2012.

20. Roßberg D, Gutsche V, Enzian S, Wick M (2002) NEPTUN 2000 – Erhebung von Daten zum tatsächlichen Einsatz chemischer Pflanzenschutzmittel im Ackerbau Deutschlands. Berichte aus der BBA, H. 98, 27 S.
21. Roßberg D (2013) Journal für Kulturpflanzen, 65 (4):141-151. doi:10.5073/JFK.2013.04.02
22. BVL (2013) Bundesamt für Verbraucherschutz und Lebesmittlesicherheit online database on plant protection products. Available at: https://portal.bvl.bund.de/psm/jsp/. Accessed 1.1.2014.
23. Sutter J (2010) Life cycle inventories of pesticides.Final report ecoinvent v2.2. Swiss Centre for Life Cycle Inventories, St. Gallen, CH.
24. Bundesamt S (2011) Düngemittelversorgung Wirtschaftsjahr 2010/2011, Wiesbaden. Available at: https://www.destatis.de/DE/Publikationen/Thematisch/IndustrieVerarbeitendesGewerbe/Fachstatistik/Duengemittel versorgungJ2040820117004.pdf?__blob=publicationFile. Accessed April 2013.
25. Jungbluth N., Chudacoff M., Dauriat A., Dinkel F., Doka G., Faist Emmenegger M., Gnansounou E., Kljun N., Spielmann M., C. S, J. S (2007) Life Cycle Inventories of Bioenergy. Final report ecoinvent data v2.0 No. 17. Swiss Centre for Life Cycle Inventories, Dübendorf, CH. .