REPORT

Compilation of emission factors for biofuels into the GAINS model script

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Report Summary

Project title
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Project sponsor
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Title and subtitle of the report

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Summary

The use of ethanol and biodiesel in the transport sector is increasing in line with the latest legislation, stimulating use of biofuels in efforts to reduce CO_2 emissions. At the same time, the aspect of effects from use of biofuel on air quality is a rather contradictory issue, which is currently being studied in many countries. The GAINS model, developed by the International Institute of Applied System Analysis (IIASA) and widely used to provide support to air quality policies, does not provide a possibility to consider emission factors for biofuels used in the transport sector (with exception for CO_2).The objective of this study is to link the biofuel share in the transport sector to available emission factors for biofuels, to provide a new emission calculation equation based on this linkage (emissions as a function of biofuel use), to introduce the equation into the GAINS Sweden script, and to compare the results obtained for several scenarios for the Swedish transport sector with different assumed levels of biofuel use. An equation, taking into consideration lower emission factors for NOx and PM from ethanol-fuelled passenger cars, has been derived and successfully compiled into the GAINS Sweden script. A generic equation applicable to other pollutants has also been derived. Calculation results indicate that introducing emission factors for biofuels does not have a significant effect on air pollutant emissions from the transport sector in Sweden. Full replacement of gasoline with ethanol for passenger cars in 2020 reduces emissions of NOx by 1.48 kt and PM by 0.06 kt, according to the baseline scenario (2009). An important prerequisite for obtaining reliable emission results in the GIAINS model is properly quantified emission factors. Further research on emission factors for biofuels is needed since currently used factors are not commonly accepted. The study has been performed within the SCARP research program.

Keyword

Biofuel, emission factor, ethanol, GAINS

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Summary

The use of ethanol and biodiesel in the transport sector is increasing in line with the latest legislation, stimulating use of biofuels in efforts to reduce CO_2 emissions. At the same time, the aspect of effects from use of biofuel on air quality is a rather contradictory issue, which is currently being studied in many countries.

The GAINS model, developed by the International Institute of Applied System Analysis (IIASA) and widely used to provide support to air quality policies, does not provide a possibility to consider emission factors for biofuels used in the transport sector (with exception for CO_2). If this possibility was introduced into the model, it would contribute to better reflection of co-benefits between air pollution and greenhouse gas mitigation.

The objective of this study is to link the biofuel share in the transport sector to available emission factors for biofuels, to provide a new emission calculation equation based on this linkage (emissions as a function of biofuel use), to introduce the equation into the GAINS Sweden script, and to compare the results obtained for several scenarios for the Swedish transport sector with different assumed levels of biofuel use.

An equation, taking into consideration lower emission factors for NOx and PM from ethanol-fuelled passenger cars, has been derived and successfully compiled into the GAINS Sweden script. A generic equation applicable to other pollutants has also been derived.

Calculation results indicate that introducing emission factors for biofuels does not have a significant effect on air pollutant emissions from the transport sector in Sweden. Full replacement of gasoline with ethanol for passenger cars in 2020 reduces emissions of NOx by 1.48 kt and PM by 0.06 kt, according to the baseline scenario (2009).

Due to the changes made in the GAINS Sweden script, it is now possible to calculate NOx emissions from the transport sector with respect to ethanol use. This feature is not provided to the users of the GAINS Europe model, owed and developed by IIASA.

An important prerequisite for obtaining reliable emission results in the GAINS model is properly quantified emission factors. Further research on emission factors for biofuels is needed since currently used factors are not commonly accepted.

The study has been performed within the SCARP research program.

Contents

Abbreviations

A	Activity data
B7	Low blend of diesel and biodiesel (7 per cent of biodiesel by volume)
CV	Calorific value
Em	Emissions
E0	Pure gasoline (100 per cent of gasoline by volume)
E100	Pure ethanol (100 per cent of ethanol by volume)
E5	Low blend of gasoline and ethanol (5 per cent of ethanol by volume)
E10	Low blend of gasoline and ethanol (10 per cent of ethanol by volume)
E40	Blend of gasoline and ethanol, 40 per cent by volume of ethanol
E85	High blend of gasoline and ethanol (≈85 per cent of ethanol by volume)
EF	Emission factor
Eff	Removal efficiency of an abatement measure
En%	Share by energy
F0	Pure fossil fuel (in general)
F100	Pure biofuel (in general)
FAME	Fatty Acid Methyl Ester (structure of biodiesel molecules)
GAINS	The Greenhouse gas – Air Pollution Interactions and Synergies model (http://gains.iiasa.ac.at/index.php/home-page)
GAS	Gas
GSL	Gasoline
HF	High blend of fossil fuel and biofuel
LCA	Life cycle analysis
LF	Low blend of fossil fuel and biofuel
MD	Medium distillates
V%	Share by volume
W	Volume share of pure biofuel in a blend
X	Implementation rate of an abatement measure

1 Introduction

The consumption of biofuels in the transport sector increases in Sweden as well as globally. Most of the biofuels are used in form of high and low blends of gasoline and ethanol or diesel and biodiesel (mostly FAME). In Sweden in 2008, ethanol (in form of E5 and E85) constituted about 3 per cent of the total energy use in the transport sector, biodiesel – 0.6 per cent, and biogas – 0.3 per cent (Rydberg et.al. 2010). The Renewable Energy Road Map 2007 sets the target of 10 per cent of biofuel use by energy in the transport sector by 2020.

New legislation, stimulating introduction of biofuels in the transport sector, is mainly targeted towards a decrease of greenhouse gas (primarily CO_2) emissions. The question of emissions of such pollutants as NOx, PM and VOC, as well as resulting impacts of emissions from biofuels on air quality (both present and future), is, however, also of high interest for scientists and policy makers.

In the GAINS model, developed by the International Institute of Applied System Analysis, there is a possibility for the user to vary shares of biofuel for certain fuels in the transport sector, namely gasoline (GSL), gas (GAS) and medium distillates (MD). This allows the user to create scenarios with different shares of biofuels and analyse the resulting changes in CO_2 emissions. In the model script, this possibility is solved by reducing activity data proportionally to the given biofuel shares, in other words, gasoline, gas, and diesel fuel consumed in the transport sector include only fossil (mineral) fuel shares (GAINS Europe – CO_2 emissions by source category). No such concept as "emission factors for biofuels" is used in the GAINS transport sector, and varying biofuel shares only affects CO_2 emissions, whereas emissions of NOx, PM and other pollutants remain unchanged.

There are several studies conducted after the introduction of E85, focusing on emission factors for NOx, PM and other pollutants from biofuel-driven vehicles. This data is quite sparse and often inconclusive; nonetheless, possible introduction of newly obtained emission factors into the script of the GAINS model could help in tentative assessments of the contribution from the use of biofuels and better reflection of interconnections (co-benefits and trade-off) between air pollution and greenhouse gas mitigation.

The objectives of this modelling study are to link biofuel share in the transport sector to available emission factors for pollutants from biofuels, to develop a new emission calculation equation based on this linkage (emissions as a function of biofuel use), to introduce the equation into the GAINS Sweden script, and to compare results obtained for several scenarios with different implied levels of biofuel use.

The report starts with an introduction, followed by a method description in Chapter 2 (including background data, system boundaries, main assumptions and the process of derivation of a new emission calculation equation considering emission factors for biofuels). Chapter 3 explains how the new equation is introduced into the GAINS Sweden script. In Chapter 4, calculation results are presented, followed by a discussion and conclusions.

2 Method

In the GAINS model, a user can set a value for the input data variable *biofuel share* (see figure 1). Although in the model this variable means energy share of pure biofuel, in practice it can be used to represent consumption of different biofuel-containing blends in different proportions.

Biofuels share in transport, %

Upload name	NEC_PRIMES_B	**Owner**	rafaj
year	Act_abb	SH_BIOF	Biofuels share, %
1990	GAS	0.00%	
1990	GSL	0.00%	
1990	MD	0.00%	
1995	GAS	0.00%	
1995	GSL	0.00%	
1995	MD	0.00%	
2000	GAS	0.00%	
2000	GSL	0.01%	
2000	MD	0.00%	
2005	GAS	0.00%	
2005	GSL	3.44%	
2005	MD	0.20%	

Figure 1. Biofuel share in the GAINS model input data

The method used to obtain a new emission equation is based on the view on available fuel blends, used by car fleet and not distinguished in GAINS, as a mixture of two standard fuel blends where each blend consists of two fuels: pure fossil fuel and pure biofuel.

In the case of ethanol and gasoline, the mixture consists of E85 and E5, a high blend and a low blend of E0 (pure gasoline) and E100 (pure ethanol), respectively (see figure 2). Consumption of other possible blends (such as E0, E100, E75, etc.) is assumed to be negligible. In the GAINS model, E85, E5, and E0 (as well as other possible blends of ethanol and gasoline) are all classified as GSL (gasoline).

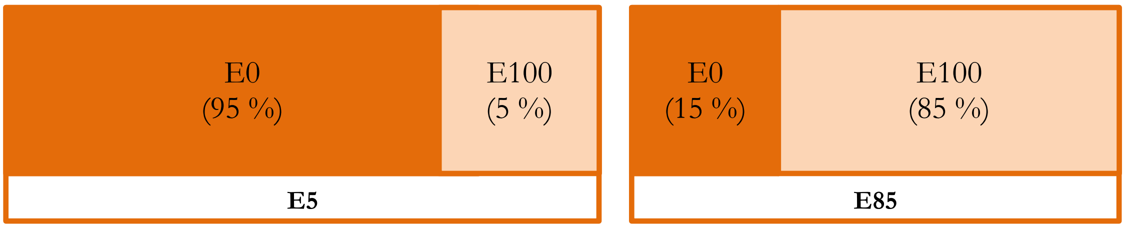

Figure 2. GSL fuel category represented as a mixture of two ethanol-gasoline blends

A new emission equation has been derived by first expressing energy share of biofuel in a fuel mixture as energy share of the high blend in the same mixture, and then calculating the resulting emissions by summarizing the emissions from the high blend with the emissions from the low blend. This is done through several steps as described below.

2.1 Background data

Research focused on emission factors for different biofuel blends is quite scarce, and the data obtained is characterized by great variability, mainly due to the diversity of the measurement methods.

For this study, data on emission factors for ethanol E85 and gasoline E5 in 2020 is taken from Fridell et al. 2010. The authors have summarized emission factors from several recent studies (2007-2009) for all major pollutants and green-house gases, for passenger cars. For several pollutants, the scaling factor between gasoline and ethanol fuelled cars is below 0.65. Thus, an assumption can be made that full substitution of gasoline E5 by ethanol E85 would significantly reduce emissions from passenger cars.

Emission factors in table 1 are given in g/km and weighted with respect to implemented Euro stages. By PM emissions in this report (as well as in the chapter discussing emission factors in Fridell et al. 2010) are meant total suspended particles, exhaust emissions only (except for the total emissions from road transport and the total national emissions of PM in Chapter 4 where non-exhaust emissions are included as well).

Table 1. Emission factors for ethanol and gasoline fuelled passenger cars, 2020 (Fridell et al. 2010)

Pollutant	**Emission factor for gasoline (E5) fuelled cars, g/km**	**Emission factor for ethanol (E85) fuelled cars, g/km**	**Scaling factor = ratio EF(E85)/EF(E5)**
NOx	0.112	0.065	0.5804
PM	0.0013	0.0008	0.6154
VOC	0.33	0.28	0.8485

It should be mentioned that, unlike for gasoline or diesel, there is no internationally accepted emission factors for biofuels, and some uncertainty thus remains.

A recent study conducted in the UK (Air Quality Expert Group 2011) summarizes emission scaling factors for different blends of bioethanol and base petrol for a range of pollutants. The results of the study include mean values for the scaling factors, but large uncertainties are identified. For instance, the scaling factor for NOx is 1.0 (no change in emissions) with the motivation that even directional change in emissions is characterized by uncertainties. Some studies suggest an increase in emissions whereas others suggest a decrease. The scaling factor for PM is assessed to be 0.4 to 0.8, depending on the blend percentage by volume.

Another large research project, specifically concentrated on effects of biofuels on emissions to air from road traffic, has been performed in the Netherlands. Based on experimental data for years 2000-2005, it is estimated that change in NOx emissions caused by use of ethanol blends varies from – 50 to +300 per cent compared to the emissions from base gasoline) (Verbeek et al. 2008). For the forthcoming years, it is noted that large variations are possible without further specification. The results of the second phase of the project indicate that the influence of ethanol blend percentage by volume on NOx and PM emissions for passenger cars can not be described by a linear function due to large variance (Verbeek et al. 2009). Emissions from biodiesel tend to be more reliable in terms of quantification, and the same study report presents minimum, average and maximum emission factors per engine technology for biodiesel.

In the present study, we use the emission factors and scaling factors presented in table 1 for ethanol E85 and gasoline E5 as best available factors at the moment, realizing that they can not be considered as conventional.

2.2 System boundaries and main assumptions

Script modifications in the GAINS Sweden are performed within the following boundaries:

- Sector: TRA_RD_4C (vehicle category passenger cars);
- Fuel: GSL (blends of gasoline and ethanol);
- Pollutants: NOx (for PM calculations are made but not the script changes);
- Years: all (1990-2030) (only 2020 for calculations).

It is assumed, for simplicity, that E85 contains 15 per cent by volume of pure gasoline E0, irrespective of the time of the year.

It is assumed in Fridell et al. 2010 that removal efficiency (percentage of emissions removed by means of a certain abatement technology) of applied Euro standard stages does not differ for ethanol fuelled and gasoline fuelled cars. In other words, scaling factors between E85 and E5 remain the same, irrespective of the implementation rates of different Euro stages. In this study, the same assumption is made.

Since the only parameter varied in the GAINS model is biofuel share, whereas activity data (energy demand), mileage and number of vehicles remain unchanged, one of the boundary conditions is that energy efficiency (PJ of energy consumed per km) is the same for any blends of gasoline and ethanol.

This assumption is partly proved by some practical data on fuel consumption. In the GAINS model, it is assumed that consumption of gasoline in passenger cars equals 0.08 l/km (Klaassen et al, 2005). Experimental data on fuel consumption per km, collected during the project BEST (http://www.best-europe.org/Pages/ContentPage.aspx?id=569), is summarized in table 2.

Calorific values of gasoline and ethanol are about 32.18 GJ/m^3 and 22.68-23.94 GJ/m^3 (depending on the time of the year), respectively (according to www.spi.se). Multiplying calorific values (GJ/m^3) by fuel consumption (l/km), we get energy efficiency of ethanol about 0.002 GJ/km and energy efficiency of gasoline about 0.004 GJ/km.

Table 2. Fuel consumption test data: gasoline and ethanol (BEST)

Car	Consumption of gasoline E5, l/100 km		Consumption of ethanol E85, l/100 km		Consumption of E85 related to E5, same car
	Interval	Mean value	Interval	Mean value	
Ford Focus	6.8-10.2	8.8	9.3-14.4	10.6	1.2
Saab FFVs	No exact data		12.5-16	13.9	1.3

The assumption of the same energy efficiency is necessary since the user would otherwise need to change either the total vehicle mileage or the total energy demand, whereas the purpose of the developed feature of the GAINS model is to get different emission results by varying only the share of biofuel, without additional adjustments in other parameters or changes in input data.

Although the model script is modified within specific boundaries, the emission calculation equation can potentially be applied to other pollutants, fuels and vehicle categories. The method is described below for the following two cases:

- General case: Fuels of consideration are any two fuel blends of the same fossil fuel and the same biofuel. These two fuel blends are not distinguished in the GAINS model. There are three fuel categories in the GAINS model transport sector corresponding to this description: GAS (meaning blends of natural gas and biogas), MD (meaning blends of diesel and biodiesel) and GSL (meaning blends of gasoline and biological analogues such as ethanol). Each of these three fuel categories can be used by different vehicles categories. The derived emission calculation equation can be used for any pollutant considered in the GAINS model, assuming that reliable emission factors for this pollutant are provided.
- Specific case: Fuels of consideration are ethanol-gasoline blends E5 and E85Pollutants of consideration are NOx and PM. Transport sub-sector (vehicle category) of consideration is passenger cars (TRA_RD_4C).

2.3 Deriving emission calculation equation

2.3.1 Step 1: From energy share of pure biofuel to volume share of pure biofuel

Input of pure biofuel in the GAINS model is given in per cent by energy. To express this value in volume shares, the following equation is used in the general case (parameters of equation 1 are explained in table 3):

$$V\%(F100) = \frac{CV(F0) * En\%(F100)}{CV(F100) + (CV(F0) - CV(F100)) * En\%(F100)} \quad (1)$$

Equation 1 is based on the additivity principle of calorific values of components in a mixture. If a mixture consists of two components, the relation between the volume share of each of these components and its energy share is described by the following equations:

$$V\%(a) = \frac{CV(b) * En\%(a)}{CV(a) + (CV(b) - CV(a)) * En\%(a)} \tag{2a}$$

$$En\%(a) = \frac{CV(a) * V\%(a)}{CV(a) + (CV(a) - CV(b)) * V\%(a)} \tag{2b}$$

where *a* and *b* are components in a two-component mixture.

Table 3. Parameters of equation 1

General case	Unit	Explanation	Specific case
F100	-	Pure biofuel	E100
F0	-	Pure fossil fuel	E0
V% (F100)	share	Share of pure biofuel by volume	V% (E100)
En% (F100)	share	Share of pure biofuel by energy	En% (E100)
CV (F100)	GJ/m^3	Calorific value of pure biofuel	21.24*
CV (F0)	GJ/m^3	Calorific value of pure fossil fuel	32.76*

* Source: Svenska Petroleum Institutet, www.spi.se.

Equation 1 is therefore a particular case of the more general equation 2a.

In the specific case, equation 1 takes the following form:

$$V\%(E100) = \frac{32.76 * En\%(E100)}{21.24 + 11.52 * En\%(E100)} \tag{3}$$

2.3.2 Step 2: From volume share of pure biofuel to volume share of high blend

One of the main assumptions of the present study is a car fleet using a mixture of two standard fuel blends consisting of two basic fuels (pure fossil fuel and pure biofuel); in this case, it is possible to define one-to-one relationship between the volume share of a pure biofuel and the volume share of a high blend in the same fuel mixture. The total volume of the fuels in the mixture can be represented as:

Volume total = Volume (F100) + Volume (F0) = Volume (HF) + Volume (LF) (4)

At the same time,

*Volume (F100) = Volume (HF) * W (HF) + Volume (LF) * W (LF)* (5) where W is a share by volume of a pure biofuel in a blend (high blend or low blend). Also,

$$Volume\ (F100)\ /\ Volume\_total = V\%\ (F100) \quad (6)$$

Following equations 4-6:

$$V\%\ (F100) = \frac{Volume(HF)*W(HF)+Volume(LF)*W(LF)}{Volume(HF)+Volume(LF)} \quad (7)$$

After expressing *Volume (HF)* through other parameters of equation 7, dividing it by *Volume total* and doing some simplifying transformations, we get the equation for volume share of a high blend as a function of volume share of a pure biofuel:

$$V\%(HF) = \frac{Volume(HF)}{Volume\_total} = \frac{V\%(F100)-W(LF)}{(W(HF)-W(LF))} \quad (8)$$

In the specific case, W (E85) = 0.85 and W (E5) = 0.05. Equation 8 thus takes the following form:

$$V\%\ (E85) = \frac{V\%(E100)-0.05}{0.8} \quad (9)$$

2.3.3 Step 3: From volume share of high blend to energy share of high blend

Energy share of a high blend is easy to get by using equation 2b:

$$En\%(HF) = \frac{CV(HF)*V\%(HF)}{CV(HF)+(CV(HF)-CV(LF))*V\%(HF)} \quad (10)$$

Calorific values of a low blend and a high blend can be calculated by using calorific values of a pure biofuel and a pure fossil fuel, and volume share W of a pure biofuel in a blend:

$$CV\ (HF\ or\ LF) = CV\ (F100)*W\ (HF\ or\ LF) + CV\ (F0) * (1-W\ (HF\ or\ LF)) \quad (11)$$

In the specific case, CV (E85) = 22.97 GJ/m^3 and CV (E5) = 32.18 GJ/m^3 (calculated using equation 11 and calorific values of E0, E100 presented in table 3).

Equation 10 takes thus the following form:

$$En\%(E85) = \frac{32.18*V\%(E85)}{32.18+9.21*V\%(E85)} \quad (12)$$

Figure 3 gives a visualisation of steps 1-3 for the specific case. Volume share of E100, volume share of E85 and energy share of E85 in the same fuel mixture (E5 and E85 used by the passenger car fleet) are represented as functions of E100 energy share (GAINS input data variable).

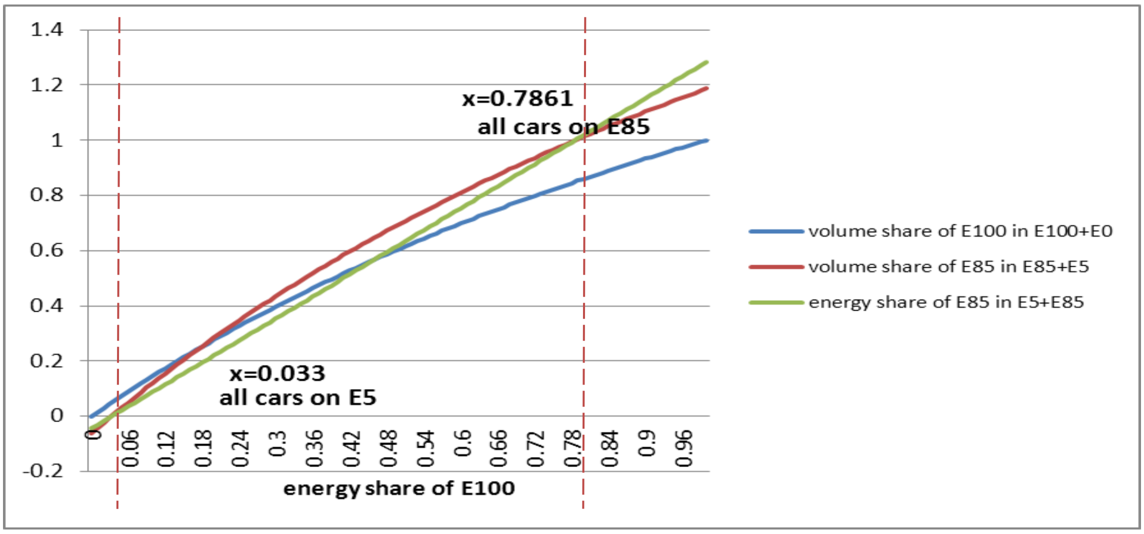

Figure 3. Shares of fuels in the fuel mixture of E5 and E85 as functions of E100 energy share

Both volume share of E100 and volume share of E85 depend on E100 energy share in a non-linear way. However, energy share of E85 is a linear function of E100 energy share, which is a consequence of additivity of volumes and calorific values.

The E85 energy share (green) line crosses the E85 volume share (brown) line in two points marked by the red dashed lines on figure 3:

- Both functions are equal to 0;
- Both functions are equal to 1.

Values of E100 energy share are in this case 0.033 and 0.7861, respectively. These two points correspond to the two boundary situations: all cars are E5 fuelled and all cars are E85 fuelled (*All E5* and *All E85* cases in Chapter 4). These are physical boundaries of the specific case: 3.3 per cent by energy (5 per cent by volume) is the minimum physically possible amount of E100 in the system where the two standard fuels are E5 and E85, and 78.61 per cent by energy (85 per cent by volume) of E100 is the maximum physically possible amount of E100 in the same system.

2.3.4 Step 4: From energy share of high blend to the final emission calculation equation

Knowing the energy share of a high blend and the scaling factor, we can now calculate input of emissions from each of the fuel blends and the total emissions from the fuel mixture.

Emissions from a high blend and a low blend, respectively, are calculated in the GAINS model as:

$$Em(HF) = A * EF(HF) * En\%(HF) = A * (EF(LF) * \frac{EF(HF)}{EF(LF)}) * En\%(HF) \quad (13)$$

$$Em(LF) = A * EF(LF) * En\%(LF) = A * EF(LF) * (1 - En\%(HF)) \quad (14)$$

where Em – emissions in kt, A – activity data in PJ, EF(HF) and EF(LF) – emission factors for a high blend a the low blend, respectively, in kt/PJ.

Total emissions are the sum of inputs from a low blend and a high blend:

$$Em = A * (EF(LF) * \frac{EF(HF)}{EF(LF)}) * En\%(HF) + A * EF(LF) * (1 - En\%(HF)) =$$

$$= \mathrm{A * EF(LF)} * (1 - En\%(HF) * (1 - \frac{EF(HF)}{EF(LF)})) \quad (15)$$

Going back consequently through the steps 3 to 1 and expressing *En% (HF)* as a function of *En% (F100)* (the GAINS input variable), we can re-write the equation 15 as follows:

$$Em = A * EF(LF) * (1 - (a * En\%(F100) + b) * (1 - \frac{EF(HF)}{EF(LF)})) \quad (16)$$

where *a* and *b* are dimensionless parameters of the linear function *a* En %(F100) +b*, corresponding to the energy share of E85 in the mixture. These two parameters are fuel-specific and depend on the calorific values of the blends and on the volume share of pure biofuel in the blends, see equation 17:

$$a = \frac{CV(F0)^2 - CV(F0)*(CV(F0) - CV(F100))*(W(LF) + W(HF)) + (CV(F0) - CV(F100))^2 * W(LF) * W(HF)}{(W(HF) - W(LF)) * CV(F0) * CV(F100)}$$

$$b = \frac{W(LF) * (CV(F0) - W(HF) * (CV(F0) - CV(F100))}{(W(HF) - W(LF)) * CV(F0)} \quad (17)$$

In the specific case of E85 and E5, a = 1.3279 and b = -0.0438, so the final emission equations for this case are as follows:

$$Em(NOx) = A * EF(E5) * (1 - (1.3279 * En\%(E100) - 0.0438) * 0.4196) \quad (18a)$$

$$Em(PM) = A * EF(E5) * (1 - (1.3279 * En\%(E100) - 0.0438) * 0.3846) \quad (18b)$$

Parameter $1 - \frac{EF(HF)}{EF(LF)}$ is fuel- and pollutant-specific and corresponds to maximum emission reduction (in shares, compared to the emissions from a low blend) achieved by total substitution of a certain low blend with a certain high blend. Thus, for NOx total substitution of gasoline E5 with ethanol E85 results in ≈ 42 per cent of emission reduction, whereas for PM the reduction will constitute ≈ 38 per cent.

The fact that the final emission equation is a linear function of energy share of pure biofuel *En% (F100)* represents high value in terms of modelling since it is totally in line with the overall principle of linearity applied to GAINS equations.

Emissions also depend linearly on energy share of a high blend, which is a consequence of the assumption of only two ethanol-gasoline blends used by passenger cars.

Appendix 1 gives an overview of all the steps of the final emission calculation derivation process.

Equation 18a for NOx is further used to modify the script of the GAINS Sweden.

3 Introduction of the emission calculation equation into the GAINS Sweden script

GAINS Sweden is a local copy of the model GAINS Europe (http://gains.iiasa.ac.at/gains/EUR/index.login?logout=1), developed by the International Institute of Applied System Analysis, re-located to the IVL server and open for modifications by IVL integrated assessment modelling research team. GAINS Sweden model script is written as SQL scripts and views.

GAINS Sweden is so far mainly used for research activities within the framework of the SCARP research program. Previously, these activities included, among others, altering scales of displaying results and varying existing model parameters outside the model to get results that is currently not possible to simulate within the model (e.g. effects of structural changes in the transport sector on emissions). The current study is the only case when the calculation script itself has been modified, including related interface changes.

3.1 Modifications in the script of GAINS Sweden

Script modifications are performed within the system boundaries described earlier: sector TRA_RD_LD4C (passenger cars), fuel GSL (gasoline + ethanol), pollutant NOx.

Script modifications for calculation of PM emissions haven't been performed but the necessary changes would follow the same pattern since the calculation equation for PM from gasoline/ethanol (equation 18b) only differs from the analogical equation for NOx (equation 18a) by one pollutant-specific parameter. Calculations of PM emissions with respect to biofuel share are performed outside the GAINS script.

Equation 18a for calculating final NOx emissions with respect to biofuels differs from the standard GAINS equation for calculating NOx emissions by the coefficient 19:

$$(1-(1.3279*En\%(E100)-0.0438)*0.4196) \qquad (19)$$

This coefficient is introduced into the model script by creating a new view *biofuel_em_adjust*. The whole equation 18a is introduced by creating a new output for emissions, which corresponds to the standard emission equation multiplied by the coefficient 19. Finally, to calculate total emissions from different Euro stages (see more details in Chapter 4) a new query table is added.

Changes in the GAINS Sweden programme script, made in connection with the incorporation of the new calculation equation 18a, are summarized in table 4.

Table 4. Modifications in the GAINS Sweden programme script

Object	**Changes**	**Formula**
View: *biofuel_em_adjust*	New view to calculate the coefficient 19 for adjusted emission factor with respect to biofuel use	(1-(1.3279*(1.-fact)-0.0438)*0.4196) as *em_adj* Variable *fact* is share of biofuel set by a user
View: *emiss_all_agg_ivl*	New output of adjusted emissions: copy of standard view for resulting emissions (*emiss_all_agg*) with join to the view *biofuel_em_adjust*.	activity * (factor_noc_abtd - rem_ef) * NVL(em_adj,1) * p.factor_display as *emiss_adj*
Query table: *emi_actTrans_IVL@NOX*	Copy of *emi_actTrans@NOX* but uses *emiss_adj* from view *emiss_all_agg_ivl* to calculate the emission sums.	

3.2 User interface modifications

Some modifications in the user interface have been done to show the resulting emissions calculated according to the new equation 18a. A new menu row *Mobile sources Biof adjust* has been introduced in addition to the standard row *NOx Emissions from Mobile Sources*, see figure 4.

Although it is possible to calculate separately emission inputs from ethanol and gasoline, the model shows the total sum – emissions from the whole *passenger cars on gasoline* category. Inputs of the two blends, shown in Appendix 2, are calculated manually.

Results obtained by calculating emissions with the new equation 18a are only seen at the level of emissions. Maps and tables, showing effects caused by emissions, are not linked to the new emission results.

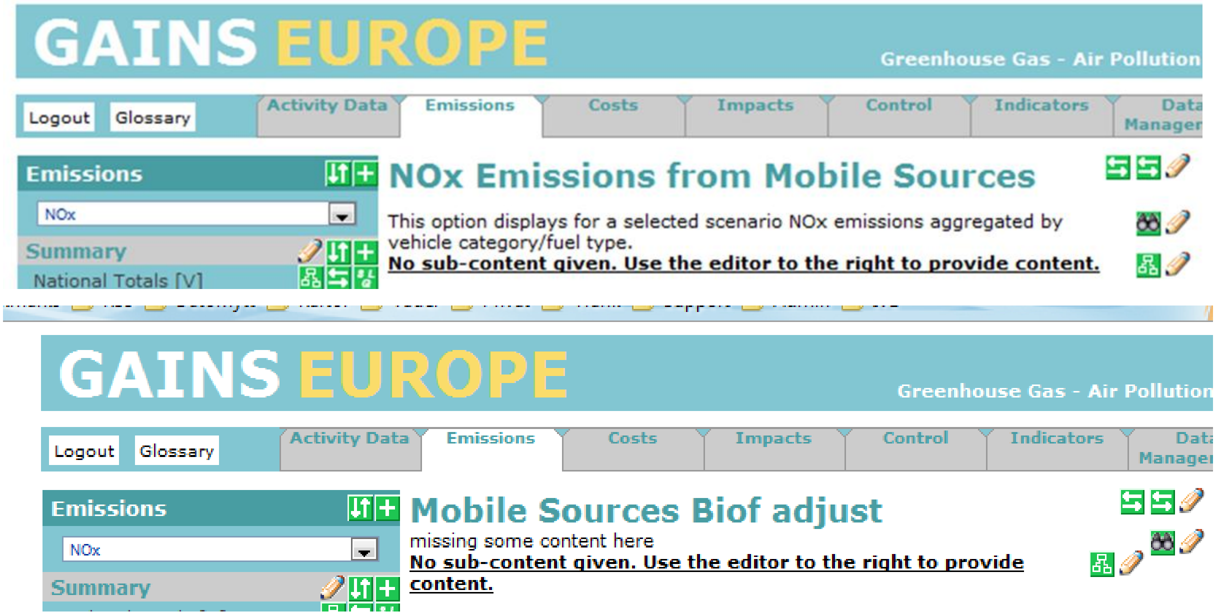

Figure 4. User interface views: standard view (above) and *Mobile Sources Biof adjust* view (below)

3.3 Limitations of the modelling cases and possibilities for validation

The fact that there are physical boundaries of the modelling case (see Chapter 2.3.3) makes it possible to create scenarios when these boundaries are exceeded by assigning to the variable *En%(E100)* values outside the interval [0.033, 0.7861]. In this case, energy share of E85 becomes either negative or >1, which does not have physical meaning. There are several possible ways to handle this problem:

- Programme control of the input data values and informing a user by an error message saying that this particular value is not possible for the chosen fuel-sector combination;
- Assigning to any values outside the interval [0.033 , 0.7861] the closest boundary values;
- No measures (currently used in the GAINS Sweden model). From mathematical point of view this situation does not represent a problem. Emissions decrease linearly depending on the energy share of E85. Both negative and exceeding 1 values of E85 energy share can be used in equations 18a, 18b. The resulting emissions would either exceed the maximum possible emissions in case all cars use gasoline or be less than minimum possible emissions if all cars use ethanol. To avoid this situation, it might be useful to warn a user by a message in the input data Excel sheet.

3.4 Euro standards: Impact on emission factors and ways to include it in calculations and modelling

In the GAINS model, emissions for each sector, fuel and pollutant are summarized by control measures in accordance with equation 20:

$$Em = \sum_i A * EF_{NOC} * (1 - Eff_i) * X_i \tag{20}$$

Here, i is a specific control measure, EF_{NOC}, or unabated emission factor, is the emission factor in kt/PJ for *No control* case – case when no control strategies are applied. Eff_i is a measure's removal efficiency in shares ($Eff_{NOC} = 0$). X_i is an implementation rate (in shares) corresponding to the part of the activity A (in PJ), covered by a control measure i. Implementation rates of all control measures (inclusive *NOC* case) gives 1.00 in sum.

For the road traffic, available control measures are mostly represented by Euro standard implementation stages. Implementation rates and pollutant-specific removal efficiencies for each Euro stage are set in the GAINS input data during scenario development. Since fossil fuels and substituting biofuels are considered as the same fuel in the GAINS model, implementation rates of Euro stages for cars using ethanol and gasoline are the same.

Equation 16 does not consider the impact of control measures on calculation results; it uses an emission factor for a low blend that can assume any abatement measure and a related scaling factor assuming the same measure. The GAINS model, however, operates with unabated emission factors EF_{NOC}, removal efficiencies Eff_i and resulting abated emission factors. Modifications in the GAINS script – introducing biofuel share dependent coefficient 19 into the emission calculation equation – are made prior to the step when control strategies are applied. After they are applied by the GAINS model, emissions in the general a case are calculated as:

$$Em = \sum_i A * EF(LF)_{NOC} *$$

$$* (1 - (a * En\%(F100) + b) * (1 - \frac{EF(HF)_i}{EF(LF)_i})) * (1 - Eff_i) * X_i \tag{21}$$

where i corresponds to a specific Euro stage or NOC (pre-Euro) case.

Since ethanol and gasoline are considered as the same fuel in the GAINS model with the same implementation rates of Euro stages, we get ratios of emission factors for all Euro stages, including stages 0-2 (not applicable to ethanol at all, since ethanol as car fuel appeared in Europe after Euro stage 3 had been introduced), with related part of emissions from these stages. This results in some overestimation of the emissions because we do not take into consideration emission reduction due to stricter standards for ethanol fuelled cars in the real life than those assigned in the model.

One of the main assumptions in this study is that the scaling factor does not depend on which Euro stage is applied to cars using different blends of fossil fuels and biofuels. This assumption is based on current knowledge and makes it possible to simplify equation 21 for the specific case for NOx as:

$$Em = \sum_i A * EF(E5)_{NOC} *$$
$$* (1 - (1.3279 * En\%(F100) - 0.0438) * 0.4196) * (1 - Eff_i) * X_i \qquad (22)$$

Equation 22 is used to calculate the final emission results, shown in the user view *Mobile Sources Biof adjusts* (see figure 4).

There is no strong scientific evidence proving this assumption; however, data on how exactly scaling factors would be changed depending on different Euro stages, is not available either.

An alternative assumption is that the ratio $\frac{EF(HF)_i}{EF(LF)_i}$ is different for each Euro stage. In that case, equation 21 is still applicable but additional changes should be introduced into the GAINS script. Coefficient 19 would be different for each Euro stage, so a separate script view for each abatement measure would be needed and the query table should be able to "collect" coefficients from each of these views.

Nonetheless, this is only possible if scaling factors are known for all Euro stages. A potential problem appearing if the scaling factors are different and at least one of them is unknown has no practical solution yet.

4 Calculation results

Equations 18a and 18b, or "biofuel adjusted" equations, are used to calculate emissions from passenger cars in Sweden for three cases for the year 2020:

- *All E85* (total substitution of gasoline with ethanol),
- *All E5* (only gasoline), and
- Baseline case for Sweden.

Scenario *National projection 2009* is chosen as baseline case since it's the most up-to-date scenario in the GAINS Sweden. This scenario assumes 19.86 per cent by energy of pure biofuel.

Some important common input data for the cases is presented in table 5.

Table 5. Scenario-specific input data for NOx and PM emission calculations, scenario *Nation projection 2009*, year 2020 (GAINS)

Energy consumption in TRA_RD_LD4C sector, GSL fuel, PJ						130
Biofuel (E100) in transport sector, % by energy						19.86
Euro stage	**Implementation rate, %**	**NOx**		**PM**		
		Removal efficiency, %	**Emission factor, kt/PJ**	**Removal efficiency, %**	**Emission factor, kt/PJ**	
NOC	0	0	0.760	0	0.0070	
Euro I	0	71	0.220	45	0.0039	
Euro II	0.6	87	0.099	45	0.0039	
Euro III	7	92	0.060	82	0.0013	
Euro IV	16.4	96	0.030	82	0.0013	
Euro V	76	97	0.023	83	0.0012	
Euro VI	0	98	0.015	84	0.0011	

The resulting emissions of NOx and PM, calculated by biofuel adjusted equations 18a, 18b and summarized by Euro stages for the three cases, are illustrated in Appendix 2. The results for NOx are calculated both in the GAINS Sweden and outside the model to ensure the quality of the script changes. Corresponding user view in the GAINS Sweden is shown in Appendix 3.

Swedish emissions for the same three cases calculated in the GAINS Europe would always be equal to 3.53 kt for NOx (see Appendix 4) and 0.159 kt for PM since the possibility to distinguish these cases is only provided in GAINS Sweden. The difference between emissions calculated by the two different equations (one with and the other without consideration of lower emission factors for biofuels) for the baseline case is 0.33 kt for

NOx and 0.014 kt for PM. This difference, as well as the input of E85 into the total emissions from the two blends in the baseline case (≈14 per cent for *Nat. projection 2009*, see Appendix 2), depends mostly on the ambition level of a chosen scenario. 19.86 per cent by energy of biofuel in 2020, assumed in the scenario *National projection 2009*, is a quite high level of ambition.

The emission reduction achieved by wider use of biofuels by passenger cars, however, does not make significant input into the total road transport emissions in Sweden, the most part of which comes from heavy duty vehicles. A quite large group of vehicles use diesel, and diesel consumption tends to increase. In the Appendix 5, total emissions of PM and NOx from Swedish road transport are represented as a function of energy share of biofuel in the ethanol-gasoline blends consumed by passenger cars in 2020. Emission decrease in the case of total substitution of gasoline E5 with ethanol E85 constitutes about 6 per cent for NOx (1.48 kt) and 1 per cent for PM (0.06 kt), in relation to the total road traffic emissions.

According to the same scenario, the total national emissions in 2020 are projected to be 111.3 kt for NOx and 60.4 kt for PM. Thus, *All E85* case would correspond to 1 per cent emission decrease in relation to the total national NOx emissions. For PM, this number is 0.1 per cent.

The more stringent Euro standards are applied to cars using fossil fuels, the less benefit in absolute numbers (kt) is achieved by substitution of a fossil fuel with a biofuel.

5 Discussion

The suggested approach of including emission factors from biofuels into the GAINS model script allows calculations of emissions from e.g. ethanol fuelled passenger cars compared to gasoline fuelled cars not only for CO_2 (as it is possible now in the GAINS Europe) but also for pollutants such as NOx and PM. Although the results indicate small differences in the resulting emissions for the particular case of ethanol and gasoline, the approach enables further exploration of co-benefits between climate and air pollution measures in the GAINS model.

One of the advantages of the approach is that the biofuel-adjusted equation is introduced into the model script by simple modifications of the original, standard GAINS equation. Fuel-specific and pollutant-specific equation parameters can be easily re-calculated (e.g. with the help of an Excel application), which makes the approach potentially applicable to other pollutants, fuel blends and vehicle categories.

One of the potential applications is adjustment of the emission calculation equations for different fuels blends in the past years. We suggest for the year 2020 that the two most commonly fuel blends are E5 and E85, building all the calculations on this assumption. However, if one wants to calculate emissions with respect to biofuels for a year when the most common gasoline fuel was pure gasoline E0, both fuel-specific and pollutant-specific equation parameters should be re-calculated for the mixture of E0 and E85. The same principle applies, for instance, to the future years if one assumes that, in accordance with the Directive 2009/30/EC, E10 will prevail.

The approach can be used for diesel fuelled cars as well. According to the Directive 2009/30/EC, B7 (7 per cent by volume of biodiesel) will most likely be implemented as a standard diesel fuel by the year 2020. If emission factors for certain pollutants significantly differ for fossil diesel and biodiesel, application of the suggested approach will probably show more significant influences on the emissions than for the case of ethanol and gasoline, mainly due to the fact that use of diesel-based fuels is expected to increase, with increased contribution of diesel fuelled cars in both road and total national emissions.

Emission factors for biofuel blends the crucial factor for obtaining reliable results, are associated with large uncertainties. We used the emission factors for NOx and PM that, according to the analysis presented in Fridell et al. 2010, are the most reliable from the few available studies on biofuels. However, as mentioned in the Chapter 2.1, most of the studies do not agree on the reliability of emission factors' quantification (this concerns both ethanol and biodiesel, not to mention less commonly used biofuels). In the latest research conducted in the UK (Air quality Expert Group 2011) and the Netherlands (Verbeek et al. 2008, Verbeek et al. 2009) the authors point out the tentative character of their results and refer to uncertainties caused by, inter alia, different biofuel feedstock and measurement methodology. They come to the same conclusion, that there is not yet sufficient data to agree on a reliable quantification of emission factors for biofuels. Therefore, for increasing reliability of the calculation results, more detailed research on emission factors is needed. Currently used emission factors are not internationally approved but judged to be the best available, and they can be easily re-calculated and corrected in the model script as soon as more accurate information on emission factors become available.

The present report addresses emission factors from both low blends and high blends of fossil fuels and biofuels. At the moment, the possibility of distinguishing inputs of these two kinds of blends into the *biofuel share* variable in the GAINS model is of more interest for Sweden than for other European countries, taking into account the efforts in Sweden to implement wider use of ethanol E85, whereas most of the other European countries concentrate on low blend alternatives. It is, however, impossible to reach "10 per cent of biofuel by energy" goal for gasoline and biodiesel, set by the Renewable Energy Road Map 2007, by using only low blends, so the possibility to calculate emissions with respect to both low blends and high blends can get more interest from other countries as well.

The two pollutants considered in this study are NOx and PM. Calculations of emissions of other pollutants can be a problematic issue due to some aspects not addressed by the GAINS model. In this relation, VOC deserves special consideration. For VOC, quantitative difference in emission factors for gasoline and ethanol is not substantial (see Fridell et al. 2010). Changes caused by increased biofuel use concern mostly the chemical speciation of VOC emissions. Studies by Fridell et al. 2010, Verbeek et al. 2008 and Air quality Expert Group 2011 suggest an increase of acetaldehyde emissions, a toxic pollutant involved in formation of tropospheric ozone, even for low blends of ethanol. For E85, also the amount of formaldehyde increases. Due to its level of generalization, GAINS considers only the total amount of emitted VOC; thus, the difference in the speciation of VOC emissions remains "unseen" and an increase in adverse effects due to formation of tropospheric ozone can not be tracked. Another reason why VOC emissions are not included in this study is that emission factors presented in Fridell et al. 2010 include evaporative emissions, which are separated in the GAINS model.

For PM, there is an evidence for different size distribution (increased number of smaller particles) for biodiesel than for fossil diesel (Air quality Expert Group 2011). This issue can not be properly taken into account in the GAINS model as long as diesel and biodiesel are considered as the same fuel with the same shares of PM size fractions in the emissions.

Another problem caused by "merging" two or more fuel blends into one category in the GAINS model is age stock of cars. Implementation rates of Euro stages in the GAINS model are the same for gasoline fuelled and ethanol fuelled cars, whereas the situation in reality is most probably different. Emissions are therefore calculated including ethanol fuelled cars corresponding to Euro stages 0 to 2 (which is not the case), which results in the underestimation of emission reduction potential of biofuel use in the model.

One issue that is realized but not fully considered during the study is that *biofuel share* of fuel categories GSL, GAS, MD in the GAINS model automatically refers not only to passenger cars but to the whole transport sector. In our calculations, we varied only biofuel share for the passenger car category, assuming that biofuel share in other transport sub-sectors does not change. In the model script, we applied the new equation to passenger cars (TRA_RD_4C) only, although according to the structure of the GAINS input data, share in other transport sub-sectors should change proportionally. The possibility to vary biofuel shares for different sub-sectors separately needs further investigation.

6 Conclusions

As a result of the present work, a new approach for compilation of emission factors for biofuels into the GAINS model script is suggested. The share of biofuel in the transport sector in the GAINS model (input data variable set by a user) is linked to the resulting emissions via emission factors for biofuels.

The script of the GAINS Sweden model is modified for the vehicle category passenger cars, fuel blends of gasoline and ethanol, and pollutant NOx. For PM, analogical calculations are done outside the model, without script modification. A generic equation, potentially applicable to other pollutants, fuel types and vehicle categories is also derived.

The new calculation equation is a linear function of biofuel energy share, which is in line with the GAINS model overall linearity principle. The equation parameters are based on scaling factors between fossil fuels and their renewable alternatives.

Calculations performed for *National projection 2009* scenario (year 2020) indicate the difference of 1.48 kt NOx when comparing the case if all passenger cars are fuelled by ethanol E85 to the case if all passenger cars are fuelled by gasoline E5. This corresponds to approximately 6 per cent of NOx emissions from road traffic or 1 per cent of national total NOx emissions in Sweden (111.3 kt). For PM, the difference constitutes 0.06 kt, which corresponds to 1 per cent of PM emissions from road traffic or 0.1 per cent of national total PM emissions in Sweden (60.4 kt).

Reported emission factors for vehicles using biofuel vary considerably. The equation parameters, currently used in the model, reflect the best available knowledge and are flexible in relation to potentially new knowledge.

Issues that need further research and clarification are identified, such as influence of Euro stage implementation on ethanol fuelled cars, separate variation of biofuel shares for different vehicle categories, more reliable quantification of emission factors, and consideration of evaporative factors and significantly changing chemical speciation of VOC.

Despite the small influence of biofuel use on the road and total national emissions of NOx and PM, the availability of the developed approach, enabling emission calculations with respect to emission factors for biofuels, contributes to better reflection of co-benefits and trade-off between air pollution and greenhouse gas mitigation in the GAINS model.

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Appendix 1. Summary of the emission equation derivation steps

Step 1: From energy share of pure biofuel to volume share of pure biofuel

General case

$$V\%(F100) = \frac{CV(F0) * En\%(F100)}{CV(F100) + (CV(F0) - CV(F100)) * En\%(F100)}$$

Specific case

$$V\%(E100) = \frac{32.76 * En\%(E100)}{21.24 + 11.52 * En\%(E100)}$$

Equation parameters

V%(F100)	share	- share of pure biofuel by volume
En%(F100)	share	- share of pure biofuel by energy
CV (F100)	GJ/m³	- calorific value of pure biofuel
CV (F0)	GJ/m³	- calorific value of pure fossil fuel

Step 2: From volume share of pure biofuel to volume share of high blend

General case

$$V\%(HF) = \frac{V\%(F100) - W(LF)}{(W(HF) - W(LF))}$$

Specific case

$$V\%(E85) = \frac{V\%(E100) - 0.05}{0.8}$$

Equation parameters

V%(F100)	share	- share of pure biofuel by volume
V%(HF)	share	- share of high blend by volume
W(LF)	share	- share of pure biofuel by volume in a low blend
W(HF)	share	- share of pure biofuel by volume in a high blend

Step 3: From volume share of high blend to energy share of high blend

General case

$$En\%(HF) = \frac{CV(HF)*V\%(HF)}{CV(HF)+(CV(HF)-CV(LF))*V\%(HF)}$$

Specific case

$$En\%(E85) = \frac{32.18*V\%(E85)}{32.18+9.21*V\%(E85)}$$

Equation parameters

V%(HF)	share	- share of a high blend by volume
En%(HF)	share	- share of a high blend by energy
CV (HF)	GJ/m^3	- calorific value of a high blend
CV (LF)	GJ/m^3	- calorific value of a low blend

Step 4: From energy share of high blend to the final emission calculation equation

General case

$$E = A*EF(LF)*(1-(a*En\%(F100)+b)*(1-\frac{EF(HF)}{EF(LF)}))$$

$a =$

$$\frac{CV(F0)^2 - CV(F0)*(CV(F0)-CV(F100))*(W(LF)+W(HF))+(CV(F0)-CV(F100))^2*W(LF)*W(HF)}{(W(HF)-W(LF))*CV(F0)*CV(F100)}$$

$$b = \frac{W(LF)*(CV(F0)-W(HF)*(CV(F0)-CV(F100))}{(W(HF)-W(LF))*CV(F0)}$$

Specific case

$$Em(NOx) = A*EF(E5)*(1-(1.3279*En\%(E100)-0.0438)*0.4196)$$

$$Em(PM) = A*EF(E5)*(1-(1.3279*En\%(E100)-0.0438)*0.3846)$$

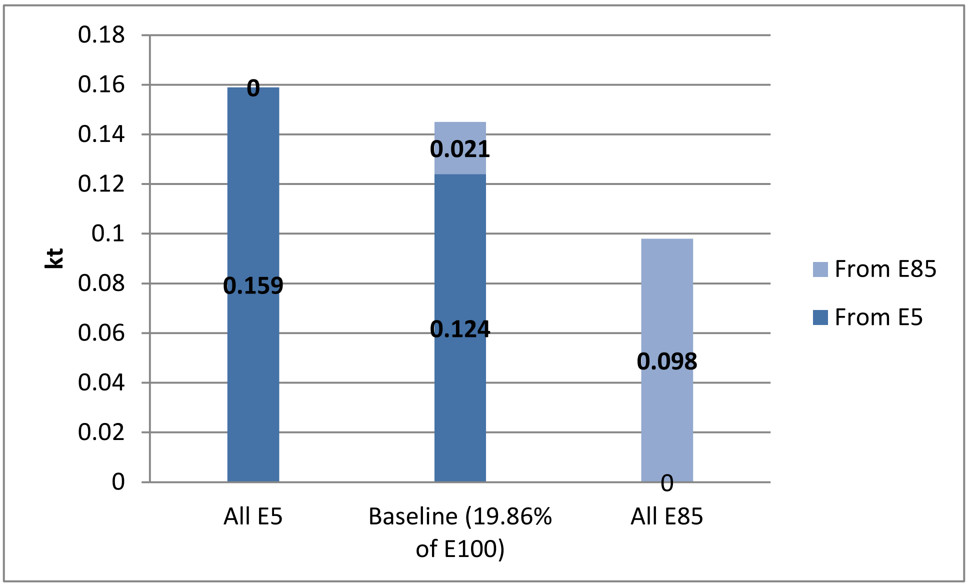
a = 1.3279, b = -0.0438

Equation parameters

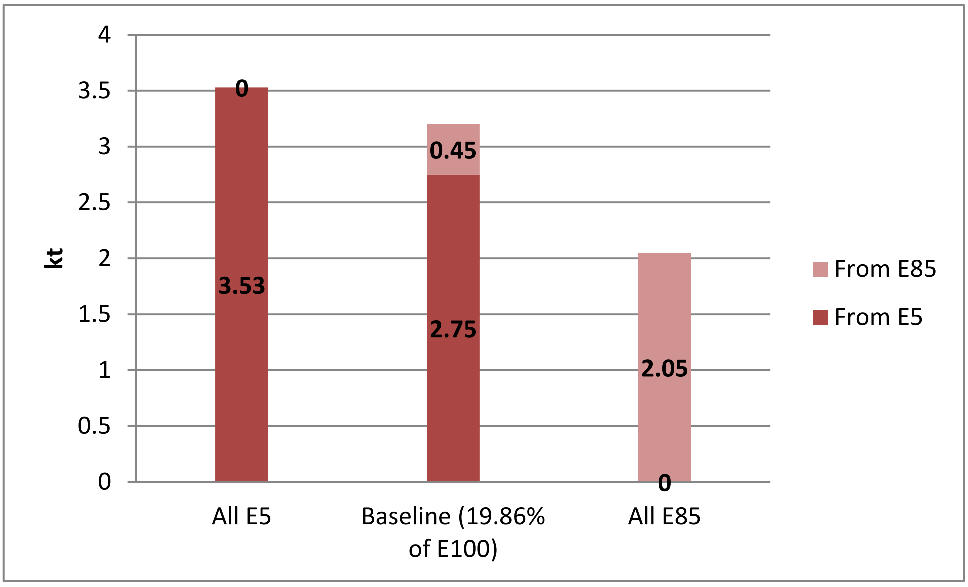
Em	kt	- emissions
A	PJ	- activity data
EF(HF)	kt/PJ	- emission factor for a high blend
EF(LF)	kt/PJ	- emission factor for a low blend
En%(F100)	share	- share of pure biofuel by energy
V%(HF)	share	- share of a high blend by volume
En%(HF)	share	- share of a high blend by energy
CV (F100)	GJ/m^3	- calorific value of pure biofuel
CV (F0)	GJ/m^3	- calorific value of pure fossil fuel
W(LF)	share	- share of pure biofuel by volume in a low blend
W(HF)	share	- share of pure biofuel by volume in a high blend

Appendix 2. Emissions of NOx and PM as a function of *biofuel share*. Sector TRA_RD_LD4C, fuel GSL, scenario *National projection 2009*, year 2020

PM

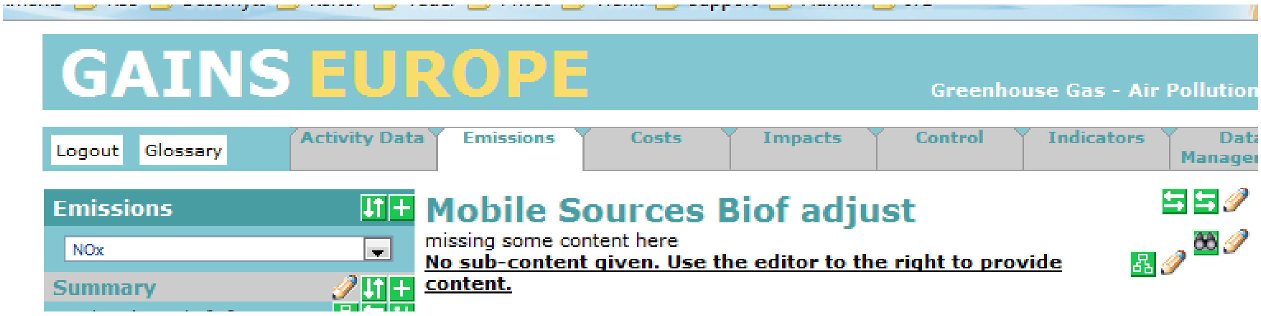


NOx



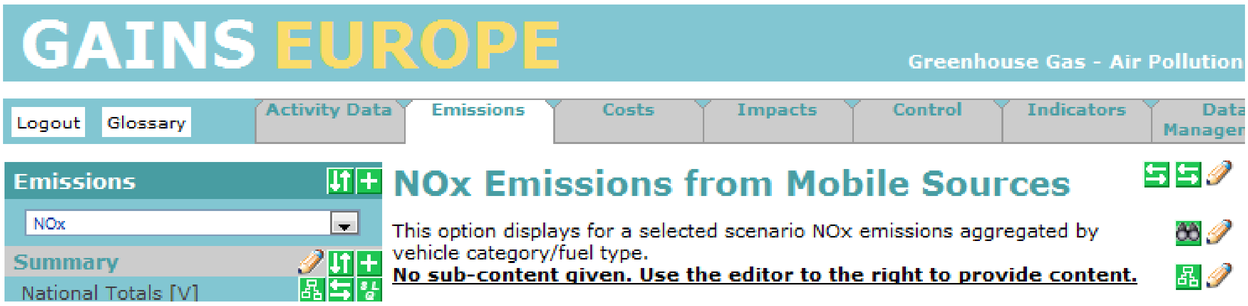
	All E5	Baseline	All E85	All E5-All E85	All E5-Baseline	From E85/Total (Baseline)
PM	0.159 kt	0.145 kt	0.098 kt	0.061 kt	0.014 kt	14.48%
NOx	3.53 kt	3.2 kt	2.05 kt	1.48 kt	0.33 kt	14.06%

Appendix 3. NOx emissions (in kt) from passenger cars calculated by biofuel-adjusted equation, user interface view: scenario *National projection 2009* (GAINS Sweden)



Natural gas (incl. other	TRA_RD_LD4C-GAS	...	0.041	...	...	0.079
Gasoline and other light	TRA_RD_LD4C-GSL	40.120	21.994	11.820	6.782	3.205
Hydrogen	TRA_RD_LD4C-H2	...	0.000	...	...	...
Liquefied petroleum	TRA_RD_LD4C-LPG	0.001	...	0.000	0.000	...
Medium distillates	TRA_RD_LD4C-MD	2.466	4.052	5.039	4.404	4.860
s-Gasoline and other	TRA_RD_LD4T-GSL	5.248	0.978	0.971	0.438	0.066
s-Medium distillates	TRA_RD_LD4T-MD	8.985	5.157	6.283	4.677	2.948
ions of oil (includes	TRA_RD_M4-GSL	0.069	0.134	0.069	0.061	0.086
	Sum	184.768	126.115	124.804	88.258	51.090

Appendix 4. NOx emissions (in kt) from passenger cars calculated by standard GAINS equation, user interface view: scenario *National projection 2009* (GAINS Europe)



-Natural gas (incl. other	TRA_RD_LD4C-GAS	...	0.041	...	...	0.079
-Gasoline and other light	TRA_RD_LD4C-GSL	39.399	22.023	12.206	7.153	3.531
-Hydrogen	TRA_RD_LD4C-H2	...	0.000	...	...	...
-Liquefied petroleum	TRA_RD_LD4C-LPG	0.001	...	0.000	0.000	...
-Medium distillates	TRA_RD_LD4C-MD	2.466	4.052	5.039	4.404	4.860
es-Gasoline and other	TRA_RD_LD4T-GSL	5.248	0.978	0.971	0.438	0.066
es-Medium distillates	TRA_RD_LD4T-MD	8.985	5.157	6.283	4.677	2.948
ions of oil (includes	TRA_RD_M4-GSL	0.069	0.134	0.069	0.061	0.086
	Sum	184.046	126.144	125.190	88.629	51.416

Appendix 5. NOx and PM emissions in Swedish road traffic as a function of biofuel share in passenger cars on gasoline-ethanol blends