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The RAINS optimization module for the Clean Air For Europe (CAFE) Programme

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Abstract

In 2005 the European Commission developed the Thematic Strategy on Air Quality (COM(2005) 446). IIASA's TAP programme has been instrumental in preparing various emission scenarios for the development of the strategy, and the optimization module of RAINS has been used extensively in the exercise. In this report we document the mathematical formulation and methodological aspects of the optimization module of RAINS.

Key words: optimization, RAINS, particulate matter

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1 Introduction

The Clean Air for Europe (CAFE) programme of the European Commission was launched in March 2001 with a Communication (COM(2001)245)). CAFE is a programme of technical analysis and policy development that underpinned the development of the Thematic Strategy on Air Pollution (COM(2005) 446) under the Sixth Environmental Action Programme. The aim of CAFE was to develop a long-term (year 2020), strategic and integrated policy advice to protect against significant negative effects of air pollution on human health and the environment. The Commission adopted the Thematic Strategy on 21 September 2005.

For the development of the Thematic Strategy IIASA's then Transbounary Air Pollution (TAP) programme had (amongst others) the task to assist in the analysis of the policies and measures related to the development of the thematic strategy and to make recommendations for most appropriate options for consideration in the CAFE work programme, as well as for the final report of the CAFE programme [Amann, 2005, Amann, 2006]. For this purpose the optimization module of the RAINS model was extended to include effects on human health of fine particulate matter ($PM_{2.5}$) in primary and secondary form, in addition to the effects of acidification, eutrophication and tropospheric ozone. In the process also all input parameters were reviewed and revised where necessary.

This report documents the optimization module of the RAINS model as it was used in the development of the Thematic Strategy. We begin by outlining the approach and detailing the essential mathematical relationships that define the optimization problem (Section 3), before addressing some alternative approaches to target setting and comparative analysis (Section 4).

Before setting out we first, however, clarify the notation used throughout this report.

2 Notation

In the remainder of this document we will use the follwing notation:

$i \in I$	the set of emitter countries (EU25 countries). It should be noted, however, that the emissions of non-EU countries are taken into account, but are considered constant and are thus absorbed into the parameters
$k \in I$	the set of receptor countries (EU25 countries)
$j \in J = J_1 \cup J_2$	the set of receptor grid cells in EU25 countries
$j \in J_1 \subset J$	grid cells in which ammonia is the limiting factor (see text)
$j \in J_2 \subset J$	grid cells in which nitrate is the limiting factor (see text)
$p \in P$	the set of relevant pollutants: SO_2, NO_x, NH_3, $PM_{2.5}$, VOC
$r \in R_{i,p}$	reduction measures/elements of the approximate cost curve in country i for pollutant p (see text)

All optmization calculations where performed using the RAINS CP_CLE Scenario for the year 2020 as a baseline. The optimization module is implemented in GAMS and uses the CPLEX solver for linear and mixed integer problems.

3 Formal Approach

3.1 Rationale and objective

In this section we present a mathematical description of the optimzation approach in RAINS. The RAINS model works with an extensive database of emission control options for different pollutants, which are represented by removal efficiencies and unit costs, and the basic idea of the optimization algorithm is to select the cost-optimal combination of control measures so that exogenouly defined environmental constraints are being met. We will now describe how the control options, the costs and the environmental impacts are represented in the model.

3.2 Marginal control cost curves

RAINS contains hundreds of technologies that can be applied in various sectors and on various activities. For the CAFE scenarios the set of available control technologies is restricted to single pollutant technologies, which means that each technology controls one and only one pollutant. This restriction justifies the use of single pollutant cost curves for the CAFE scenarios. Multi-pollutant technologies (such as Euro standards in the transportation sector which control SO_2, NO_x and $PM_{2.5}$ emissions) are introduced at a later stage of the scenario development in the form of package solutions (e.g. Euro 4 vs Euro 5/6 standards). These are assumed exogenously without them being subject to the optimization procedure. In this way it is possible to run sensitivity cases and estimate the relative cost-effectiveness of the Euro standards compared to the most cost-effective set of measures in other sectors.

Single pollutant reduction technologies $t = t(i, a, p)$ in a given country i for a given activity a and pollutant p are characterized by their removal efficiency $\text{eff}_{a,t,p}$, marginal cost $\text{MC}_{i,a,t,p}$ and its abatement potential $x^{\max}_{i,a,t,p}$. The marginal cost is calculated as

$$\text{MC}_{i,a,t,p} = \frac{uc_{i,a,t} - uc_{i,a,t-1}}{\text{EF}_{i,a,p}(\text{eff}_{a,t,p} - \text{eff}_{a,t-1,p})} \tag{1}$$

where $\mathrm{EF}_{i,a,p}$ is the unabated emission factor of pollutant p, and $uc_{i,a,t}$ is the unit cost (per unit of activity) of technology t applied to activity a.

In the RAINS database for each pollutant and each region there are typically several hundred control technologies documented, many of which are already used in baseline projections. However, typically several dozens of technologies per pollutant have additional application potential over the baseline. Yet for some of these technologies this potential is negligible, or they have marginal costs that are almost identical to other technologies that apply to the same pollutant, so the first step we took for the CAFE optimization approach to improve computational efficiency was to generate cost curves that approximate the exact cost curves very well, but only contain 20-30 piecewise-linear sections.

The decision variables of the optimization are then simply the emission reductions $x_{i,r,p}$ with

$$0 \leq x_{i,r,p} \leq x_{i,r,p}^{\max} \tag{2}$$

of pollutant p in country i with the reduction technology r, having marginal costs $\mathrm{MC}_{i,r,p}$. Note that with the approximate cost curves, r does not necessarily represent a single technology, but possible a mix of technologies $\{(a,t)\}$ with similar marginal costs, but the set of r's is ordered such that $\mathrm{MC}_{i,r,p} < \mathrm{MC}_{i,r+1,p}$.

The marginal costs are thus collected into a marginal abatement cost curve with start point Current Legislation (CLE) or baseline emissions ($\mathrm{CLE\_emissions}_{i,p}$) and end point Maximum Technically Feasible Reduction Scenario ($\mathrm{MTFR\_emissions}_{i,p}$). For the MTFR scenario we have $x_{i,r,p} = x_{i,r,p}^{\max}$), i.e. all technologies on the approximate cost curve are applied to their maximum possible extent so that:

$$\mathrm{MTFR\_emissions}_{i,p} = \mathrm{CLE\_emissions}_{i,p} - \sum_{r \in R_{i,p}} x_{i,r,p}^{\max} \tag{3}$$

A feasible emission level $\mathrm{emissions}_{i,p}$ of pollutant p in country i can thus be written as

$$\mathrm{emissions}_{i,p}^{*} = \mathrm{CLE\_emissions}_{i,p} - \sum_{r=1}^{r^*} x_{i,r,p} - \delta \tag{4}$$

where r^* is an integer such that

$$\mathrm{CLE\_emissions}_{i,p} - \sum_{r=1}^{r^*} x_{i,r,p} \geq \mathrm{emissions}_{i,p}^{*} \tag{5}$$

and

$$\mathrm{CLE\_emissions}_{i,p} - \sum_{r=1}^{r^*+1} x_{i,r,p} \leq \mathrm{emissions}_{i,p}^{*} \tag{6}$$

In order to reach the emission level $\mathit{emissions}_{i,p}^{*}$ the technology r^*+1 is typically not applied to the maximal possible extent: having applied technology r^*, only a further reduction by δ is needed (cf. (4)) with:

$$\delta = \delta(i,p,r^*,\{x_{i,r,p}^{\max}\},\mathrm{CLE\_emissions}_{i,p},\mathrm{emissions}_{i,p}^{*}) \tag{7}$$

$$= \mathrm{CLE\_emissions}_{i,p} - \mathrm{emissions}_{i,p}^{*} - \sum_{r=1}^{r*} x_{i,r,p} \tag{8}$$

For the total cost of reaching the emission level $\text{emissions}^*_{i,p}$ we thus find

$$\text{cost}(\text{emissions}^*_{i,p}) = \sum_{r=1}^{r^*} \text{MC}_{i,r,p} \cdot x^{\max}_{i,r,p} + \text{MC}_{i,r^*+1,p} \cdot \delta \tag{9}$$

with δ given in (8).

3.3 The Objective Function

After these preliminaries on cost curves we now return to the rationale of the optimization approach. The objective of the scenario exercise is to develop cost-optimal solutions under given enviromental constraints. Thus the objective function is defined by:

$$\text{Objective Function} = \text{Total Cost}_{\text{EU25}} = \sum_{i \in \text{EU25}} \sum_{p \in P} \sum_{r \in R_{i,p}} \text{MC}_{i,r,p} \cdot x_{i,r,p} \tag{10}$$

An alternative formulation, minimizing environmental impacts for a given amount of money, is not considered useful in the context of multiple environmental effects.

It should be clear that in a cost minimization scheme, the formulation (10) is fully consistent with (9): though the sum over r in (10) runs over all $r \in R_{i,p}$, the fact that the reduction options are ordered by their marginal cost ensures that for given target level $\mathit{emissions}^*_{i,p}$ the sum over r on the right hand side of (10) reduces to (9) when costs are minimized.

3.4 Environmental Impacts

For this exercise we study four different impacts of the five pollutants (SO_2, NO_x, NH_3, $PM_{2.5}$, VOC):

- **Acidifcation.** The impact indicator used is *average accumulated exceedance* and is a linear function:

$$\begin{aligned} \text{acid}_k \;=\; & \sum_{i \in I} tnac_{i,k} \cdot \text{emissions}_{i,\text{NO}_x} + \sum_{i \in I} taac_{i,k} \cdot \text{emissions}_{i,\text{NH}_3} \\ & + \sum_{i \in I} tsac_{i,k} \cdot \text{emissions}_{i,\text{SO}_2} + kac_k \end{aligned} \tag{11}$$

  where $tnac_{i,k}$, $taac_{i,k}$, and $tsac_{i,k}$ are transfer coefficients and kac_k are constants that are used to calibrate the linear approximation.

- **Eutrophication.** The impact indicator used is *average accumulated exceedance* and is a linear function:

$$\text{eutr}_k = \sum_{i \in I} tnec_{i,k} \cdot \text{emissions}_{i,\text{NO}_x} + \sum_{i \in I} taec_{i,k} \cdot \text{emissions}_{i,\text{NH}_3} + kec_k \tag{12}$$

  where $tnec_{i,k}$ and $taec_{i,k}$ are transfer coefficients and kec_k are constants that are used to calibrate the linear approximation.

- **Ground level ozone.** The impact indicator used is *SOMO35*. SOMO35 is calculated as the sum of the daily eight-hour maximum ozone concentrations in excess of a 35 ppb threshold, integrated over the full year. In linearized form

$$\text{SOMO35}_k = \sum_{i \in I} tno_{i,k} \cdot \text{emissions}_{i,\text{NO}_x} + \sum_{i \in I} tvo_{i,k} \cdot \text{emissions}_{i,\text{VOC}} + ko_k \tag{13}$$

where $tno_{i,k}$ and $tvo_{i,k}$ are transfer coefficients and ko_k are constants that are used to calibrate the linear approximation.

- **Years of Life Lost (YOLL)** The loss of life expectancy (for the population above age 30) can be linearly related to $PM_{2.5}$-concentration [Rabl,2006]:

$$\text{YOLL(EU25)} = \sum_{k \in EU25} \sum_{j \in J} \text{PM}_{2.5}\text{-concentration}_{\text{cell}_j} \cdot \text{D}_k \cdot \text{pw}_{j,k} \tag{14}$$

where $\text{pw}_{j,k}$ is the population weight of grid cell j in country k, and the country-specific parameter D_k can be derived from the Cox Proportional Hazards Model, taking into account the changes in life expectancy for each cohort [Mechler, 2002]. The $\text{PM}_{2.5}\text{-concentration}_{\text{cell}_j}$ is calculated for each grid cell, where we distinguish *ex ante* those grid cells in which ammonia ($j \in J_1$) or nitrate ($j \in J_2$) is the limiting factor in the formation of ammonium nitrate. This distinction is useful because the formation of secondary $\text{PM}_{2.5}$ is determined by the availability of its precursors and for the optimization we can thus reduce a combination of *min* and *max* operators to a single *max* operator, see (19). We can write in compact form:

$$\text{PM}_{2.5}\text{-concentration}_{\text{cell}_j} = \text{pPM}^a_{2.5,j} + \text{S}^a_j + \text{AN}^S_j + \text{AN}^W_j + k^j_3 \tag{15}$$

where the individual terms are

  - annual mean primary $\text{PM}_{2.5}$ concentration

$$\text{pPM}^a_{2.5,j} = \sum_{i \in I} \pi^a_{i,j} \cdot \text{emissions}_{i,\text{PM}} \tag{16}$$

  - annual mean sulphate $[\text{SO}_4]$ concentration

$$\text{S}^a_j = \sum_{i \in I} \sigma^a_{i,j} \cdot \text{emissions}_{i,\text{SO}_2} \tag{17}$$

  - summer mean ammonium nitrate $[\text{NH}_4\text{NO}_3]^S$

$$\text{AN}^S_j = \frac{6}{12} \cdot \sum_i \alpha^S_{i,j} \cdot \text{emissions}_{i,\text{NH}_3} + \frac{6}{12} \cdot \sum_i \nu^S_{i,j} \cdot \text{emissions}_{i,\text{NO}_x} \tag{18}$$

  - winter mean ammonium nitrate $[\text{NH}_4\text{NO}_3]^W$

$$\text{AN}^W_j = \begin{cases} \frac{6}{12} \cdot \max(0, \text{rem\_NH}_{3,j}) & : \quad \text{for } j \in J_1 \\ \frac{6}{12} \cdot \sum_{i \in I} \rho_j \cdot \nu^W_{i,j} \cdot \text{emissions}_{i,\text{NO}_x} & : \quad \text{for } j \in J_2 \end{cases} \tag{19}$$

and k^j_3 is the constant that is used to calibrate the linear approximation (15) which includes, also the mineral component of $\text{PM}_{2.5}$, and ρ_j is a dimensionless scaling factor that takes into account the water content and is used to calibrate the linear relationship. The auxiliary variable $\text{rem\_NH}_{3,j}$ is representing the ammonia that is remaining after reaction with sulphate: where

$$\text{rem\_NH}_{3,j} = \sum_{i \in I} \varepsilon_j \cdot \alpha^W_{i,j} \cdot \text{emissions}_{i,\text{NH}_3} - \frac{14}{32} \sum_{i \in I} \varepsilon_j \cdot \sigma^W_{i,j} \cdot \text{emissions}_{i,\text{SO}_2} \tag{20}$$

and here ε_j is a dimensionless scaling factor that takes into account the water content and is used to calibrate the linear relationship.

Equation (14) describes the EU25-YOLL function as a function of national emissions of SO_2, NO_x, $PM_{2.5}$ and NH_3. As an intermediate step the $PM_{2.5}$ concentration in each grid cell is calculated using Eq. (15), so that the total loss of life expectancy is a country-to-cell transfer relation followed by a cell-to-EU25 relation. This turns the optimization into a high-dimensional mixed-inter problem because the formulation (19) requires the use of a binary variable in each grid cell (of which there are several thousands) and this is a computationally demanding procedure.

For this reason, the sum over j in (14) is performed first and the following simplification is made:

$$\sum_{j \in J_1} \max\left(0, \text{rem\_NH}_{3,j}\right) \longrightarrow \max(0, \sum_{j \in J_1} \text{rem\_NH}_{3,j}) \tag{21}$$

With this the transfer coefficients and parameters can be aggregated, so that the resulting relationship between the emissions and the loss in life expectancy in EU25 is direct and only implicitly calculated through the grid cells. An error is thus introduced for cells in which $\text{rem\_NH}_{3,j}$ is negative. In future scenarios this error will be reduced by appropriate ex ante analysis of the possible sign of this variable.

4 Optimization

In the optmization approach for the CAFE scenarios we minimize the total costs (10) subject to environmental constraints, which we will discuss below, and technology specific constraint, reflected in the cost curves represented by (2).

4.1 Environmental target setting

Environmental constraints are imposed by defining ceilings for environmental impact indicators:

$$\begin{aligned}
\text{acid}_k &\leq (\text{acidification ceiling})_k && \text{(22a)}\\
\text{eutr}_k &\leq (\text{eutropication ceiling})_k && \text{(22b)}\\
\text{SOMO35}_k &\leq (\text{SOMO35 ceiling})_k && \text{(22c)}\\
\sum_{k \in EU25} \text{country_YOLL}_k &\leq \text{YOLL ceiling} && \text{(22d)}
\end{aligned}$$

where the values for the ceilings are typically determined using a gap closure approach (see next section). Note that the ceiling for the YOLL indicator is implied at the EU25 level, whereas the other indicators are constrained at the country level. As an alternative target setting approach to Eq. (22d) one can also introduce a ceiling on $PM_{2.5}$ concentrations at the grid cell level j

$$\text{PM}_{2.5}\text{-concentration}_{\text{grid}_j} \leq \text{PM}_{2.5}\text{-concentration ceiling} \tag{23}$$

where equity considerations suggest that the concentration ceiling is independent of the index j, i.e. holds in every grid cell. However, in this approach only $PM_{2.5}$-concentration ceilings can be selected that are higher than the concentration level of the worst polluted grid cell in the MTFR scenario. Also from the point of view of health benefits (in a country or in EU25), this method of target setting turns out to be neither cost-effective (cost per health benefit) nor equitable (e.g. in terms of health benefit per capita, or cost per capita etc).

4.2 Gap closure approach

The gap closure approach is used to determine target values on the effect indicators. The underlying idea is to achieve a uniform relative improvement across all k in (22a)-(22c), that is all receptor countries (Since (22d) is not indexed by receptor countries, the gap closure approach in this case can be interpreted as setting a single target value, and *vice versa*). In contrast to previous analysis performed with the RAINS model in the development of the National Emissions Ceilings Directive of the European Commission for the year 2010 the gap closure concept for the CAFE program only covers the effect range between CLE and MTFR, and not between base year effect and zero effect:

$$X \text{ ceiling} = (\text{CLE value of } X) - \text{GC}(X) \cdot (\text{CLE value of } X - \text{MTFR value of } X) \quad (24)$$

where X can stand for YOLL, acidification, eutrophication or SOMO35 and GC(X) is the gap closure percentage applied to the indicator X, and its range is $0\% - 100\%$. The CLE and MTFR values of X are calculated by inserting the CLE and MTFR emissions into the effect definitions (11)-(15), respectively. This gap closure approach seems to be restricted compared to the approach previously employed; however, this restriction is only an apparent one. In fact, the restriction ensures that any value between 0% and 100% is feasible and hence all feasible effect improvements can be reached. Naturally, different gap closure approaches may, and typically will, result in different national emission allocations.

4.3 Configurations

Minimizing the objective function (10) subject to (2) is a well-defined but trivial task ($x_{i,r,p} = 0$), as the CLE solution is being recovered as cost optimal. Only when one or more constraints on impacts (22) are added to the problem we do obtain non-trivial results. For the CAFE scenarios various combinations of constraints (22) were calculated to estimate the marginal cost of an additional constraint, given that constraints on one or more other impacts. For example, first the minimal cost response to impact ceilings on acidification, eutrophication and SOMO35 was calculated, and it came out at, say, 8bln Euro per year. Then a constraint on YOLL was added and the cost-optimal solution calculated, which costs, say 9bln Euro per year, so that the additional constraint can be said to cost 1bln Euro per year. Marginal costs of impact constraints are useful indicators as they reflect more accurately the projected control costs for an additional constraint against the background of other constraints.

4.4 Sensitivity analysis

Various types of sensitivity analysis were performed:

- Euro standards. Two alternative CLE scenarios were used: one assuming that Euro 5/6 will be in place in 2020, and one that assumes the implementation of Euro 4 only. Consistency is ensured by shifting the cost curves for the relevant pollutants and with them the MTFR emissions.

- Reductions of the emissions from ships in international waters are not included in the optimization. Rather, as a sensitivity case we considered a family of scenarios for which ship emissions are subject to tighter controls than in the baseline.

- In addition to the analysis based on energy scenarios generated with the PRIMES model, we have also performed a study of scenarios that were provided by national

experts (so-called NAT scenarios, which were developed in process of bilateral consultations with EU member states). For those member states that did not provide a national baseline scenario, the PRIMES baseline scenario) was retained.

- Impact of secondary PM. In all of the analysis above it was assumed that both the primary and secondary $PM_{2.5}$ contributions are responsible for loss of human life, though this is uncertain. In a series of sensitivity runs we have assumed that only the primary part of $PM_{2.5}$ contributes to loss of life, i.e. we set the contribution of secondary PM to zero, calculated the baseline figures and applied the same target setting procedure (gap closure) in order to obtain comparable ambition levels.

- In an earlier part of the exercise we also explored the possibility to impose universal $PM_{2.5}$ concentration ceiling at the grid cell level. There are, however, a number of important limitations to this approach, the most significant being that this universal concentration ceiling that is imposed in all grid cells can only be so ambitious as is feasible in the most polluted cells, or rather in those where reductions to low levels are hardest to achieve. In other words, while binding in a few grid cells, the concentration ceiling will be higher than the concentration levels in the CLE scenario in many grid cells. The cost and feasibility of not exceeding the concentration ceiling is thus largely driven by the constraints in a minority of the grid cells. That this is not an efficient approach to EU-wide air pollution control should be obvious. Our calculations also indicate that the approach would also not be more equitable (using standard equity indicators).

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Appendix

Symbol and its derivation	Description	Unit
$\pi^a_{i,j} = \frac{\Delta_{\mathrm{PM}_{2.5i}}(pm25_j)}{(0.15 \times \overline{\mathrm{PM}_{2.5i}})}$	annual average base scenario: CLE	$\mu g(PM)\, m^{-3}/kt(PM)$
$\sigma^a_{i,j} = \frac{\Delta_{\mathrm{SO}_{2i}}(3 \times so4^w_j + pm25^s_j + pm25\_\mathrm{H_2O}^a_j)}{(0.15 \times \overline{\mathrm{SO}_{2i}})}$	annual average base scenario: CLE	$\mu g(PM)\, m^{-3}/kt(SO_2)$
$\alpha^s_{i,j} = \frac{\Delta_{\mathrm{NH}_{3i}}(pm25_j + pm25\_H_2O_j)}{(0.15 \times \overline{\mathrm{NH}_{3i}})}$	summer (May-Oct) base scenario: CLE	$\mu g(PM)\, m^{-3}/kt(NH_3)$
$\nu^s_{i,j} = \frac{\Delta_{\mathrm{NO}_{xi}}(pm25_j + pm25\_H_2O_j)}{(0.15 \times \overline{\mathrm{NO}_{xi}})}$	summer (May-Oct) base scenario: 'SN50'	$\mu g(PM)\, m^{-3}/kt(NO_x)$
$\alpha^w_{i,j} = \frac{\max\Delta_{\mathrm{NH}_{3i}}(\mathrm{NH}_{4j})}{(0.15 \times \overline{\mathrm{NH}_{3i}})}$	winter (Nov-Apr) maximum delta over various scenarios	$\mu g(PM)\, m^{-3}/kt(NH_3)$
$\sigma^w_{i,j} = \frac{\Delta_{\mathrm{SO}_{2i}}(so4^w_j)}{(0.15 \times \overline{\mathrm{SO}_{2i}})}$	winter (Nov-Apr) base scenario: CLE	$\mu g(PM)\, m^{-3}/kt(SO_2)$
$\nu^w_{i,j} = \frac{\max\Delta_{\mathrm{NO}_{xi}}(\mathrm{NO}_{3j})}{(0.15 \times \overline{\mathrm{NO}_{xi}})}$	winter (Nov-Apr) maximum delta over various scenarios	$\mu g(PM)\, m^{-3}/kt(NO_x)$

Table 1: Parameters used in the $\mathrm{PM}_{2.5}$ concentration calculation