REACT4C – Cost functions

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1 Cost functions – metrics

AGWP and AGTP for a species x are defined as:

$$AGWP_x = \int_0^H F_x(t)\,dt \tag{1}$$

$$AGTP_x = \int_0^H F_x(t)\,R(H-t)\,dt \tag{2}$$

where $F_x(t)$ is the forcing and $R(H-t)$ is the response function given by Eqn. (A2) in Fuglestvedt et al. (2010) (F2010 from now):

$$R(\xi) = \sum_{j=1}^{2} \frac{c_j}{d_j} \exp\left(\frac{-\xi}{d_j}\right) \tag{3}$$

The forcing put out from the model is adjusted to annual mean, i.e. integrated forcing of the pulse emission. In essence, this is AGWP for the time period integrated over. To calculate AGWP and AGTP for different time horizons, we assume the forcing to be a pulse of amplitude A_x, with an exponential lifetime τ_x. The annual mean radiative forcing $\overline{F_x}$ is then:

$$\overline{F_x} = \int_0^1 A_x \exp\left(-\frac{t}{\tau_x}\right) dt \tag{4}$$

$$= A_x\tau_x \left[1 - \exp\left(-\frac{1}{\tau_x}\right)\right] \tag{5}$$

From this we find the assumed initial pulse A_x.

1.1 AIC

For AIC, with a short response lifetime τ_{aic}, we get from Eqn. 5:

$$A_{aic} = \frac{\overline{F_{aic}}}{\tau_{aic}\left(1 - e^{-\frac{1}{\tau_{aic}}}\right)} \approx \frac{\overline{F_{aic}}}{\tau_{aic}} \tag{6}$$

Having the pulse A_{aic} and its exponential decay rate, we have the forcing as a function of time:

$$F_{aic}(t) = A_{aic}\,e^{-\frac{t}{\tau_{aic}}} \tag{7}$$

and we calculate AGWP using Eqn. (1):

$$AGWP_{aic} = \int_0^H F_{aic}(t)\,dt \tag{8}$$

$$= A_{aic}\tau_{aic}\left(1 - e^{-\frac{H}{\tau_{aic}}}\right) \tag{9}$$

AGTP is defined by Eqn. (2), and solving for this using Eqn. (7) and Eqn. (3), we get Eqn. (A4) in F2010:

$$AGTP_{aic} = \sum_{j=1}^{2} \frac{A_{aic}\,\tau_{aic}\,c_j}{\tau_{aic} - d_j}\left(e^{-\frac{H}{\tau_{aic}}} - e^{-\frac{H}{d_j}}\right) \tag{10}$$

1.2 O_3 – short-lived

From the model we also have O_3 annual mean forcing, i.e. integrated forcing for one year. In general, the short-lived O_3 response reaches maximum after a certain time ε, and then decays. We consider two possibilities:

1. Approximate by assuming an instant peak of A_{O3}, then decay according to lifetime.
2. Exponential increase ($\frac{1-e^{-t/b}}{1-e^{-\varepsilon/b}}$) until $t = \varepsilon$, with maximum A_y, followed by decay according to lifetime.

The two options will give slightly different $F_{O3}(t)$, but as we will show, option 1 is a good approximation because most of the signal occurs during the first year.

option 1
Assuming $F_{O3}(t)$ decaying exponentially from A_{O3}, we get:

$$F_{O3}(t) = A_{O3}\,e^{-\frac{t}{\tau_{O3}}} \tag{11}$$

And similarly to AIC in Eqn. (6), we get from the integrated forcing $\overline{F_{O3}}$ for the first year:

$$A_{O3} = \frac{\overline{F_{O3}}}{\tau_{O3}\left(1 - e^{-\frac{t}{\tau_{O3}}}\right)} \approx \frac{\overline{F_{O3}}}{\tau_{O3}} \tag{12}$$

option 2
The second option – assuming a delay in the forcing peak, requires knowledge of when the peak occured. Out test assumption is that the signal rises from zero to A_y at $t = \varepsilon$ within the first year, as a function of $1 - e^{t/b}$:

$$F_{O3,2}(t) = A_y \frac{1 - e^{-\frac{t}{b}}}{1 - e^{-\frac{\varepsilon}{b}}} \qquad \text{for } 0 \le t \le \varepsilon \tag{13}$$

$$F_{O3,2}(t) = A_y\,e^{-\frac{t}{\tau_{O3}}} \qquad \text{for } \varepsilon < t \tag{14}$$

We assume $b = 0.025\varepsilon$, so the response up to maximum is fairly quick, and integrate the forcing for 1 year, to get $\overline{F_{O3}}$:

$$\begin{aligned}\overline{F_{O3}} &= \int_0^1 F_{O3,2}(t)\,dt \\ &= \frac{A_y}{1-e^{-\frac{\varepsilon}{b}}}\int_0^{\varepsilon} 1-e^{-\frac{t}{b}}\,dt \\ &+ A_y \int_{\varepsilon}^{1} e^{-\frac{t}{\tau_{O3}}}\,dt \qquad (15)\\ &= \frac{A_y}{1-e^{-\frac{\varepsilon}{b}}}\left|t+be^{-\frac{t}{b}}\right|_0^{\varepsilon} \\ &- A_y\,\tau_{O3}\left|e^{-\frac{t}{\tau_{O3}}}\right|_{\varepsilon}^{1} \\ &= A_y\frac{\left(\varepsilon+be^{-\frac{\varepsilon}{b}}-b\right)}{1-e^{-\frac{\varepsilon}{b}}} \\ &+ A_y\,\tau_{O3}\left(e^{-\frac{\varepsilon}{\tau_{O3}}}-e^{-\frac{1}{\tau_{O3}}}\right) \qquad (16)\end{aligned}$$

We solve Eqn. (16) for A_y:

$$A_y = \frac{\overline{F_{O3}}}{\frac{\left(\varepsilon+be^{-\frac{\varepsilon}{b}}-b\right)}{1-e^{-\frac{\varepsilon}{b}}}+\tau_{O3}\left(e^{-\frac{\varepsilon}{\tau_{O3}}}-e^{-\frac{1}{\tau_{O3}}}\right)} \qquad (17)$$

Error estimates
The value of A_y could be considered "more correct" compared to our choice of A_{O3}. However, we want to show that the assumption of an instant peak of the latter is valid for the integral (i.e. area below the curve), so we integrate AGWP for $H = 20$ years for both methods:

$$\begin{aligned}AGWP_1 &= \int_0^H A_{O3}\,e^{-\frac{t}{\tau_{O3}}}\,dt \\ &= A_{O3}\,\tau_{O3}\,(1-e^{-\frac{H}{\tau_{O3}}}) \qquad (18)\\ AGWP_2 &= \frac{A_y}{1-e^{-\frac{\varepsilon}{b}}}\int_0^{\varepsilon} 1-e^{-\frac{t}{b}}\,dt \\ &+ A_y\int_{\varepsilon}^{H} e^{-\frac{t}{\tau_{O3}}}\,dt \qquad (19)\\ &= A_y\frac{\left(\varepsilon+be^{-\frac{\varepsilon}{b}}-b\right)}{1-e^{-\frac{\varepsilon}{b}}} \\ &+ A_y\,\tau_{O3}\left(e^{-\frac{\varepsilon}{\tau_{O3}}}-e^{-\frac{H}{\tau_{O3}}}\right) \qquad (20)\end{aligned}$$

Similarly, we integrate for AGTP:

$$\begin{aligned}AGTP_1 &= \int_0^H A_{O3}\,e^{-\frac{t}{\tau_{O3}}}\,R(H-t)\,dt \\ &= \sum_{j=1}^{2}\frac{A_{O3}\,\tau_{O3}\,c_j}{\tau_{O3}-d_j}\left(e^{-\frac{H}{\tau_{O3}}}-e^{-\frac{H}{d_j}}\right)\end{aligned}$$

$$\begin{aligned}AGTP_2 &= \int_0^{\varepsilon} A_y\,\frac{1-e^{-\frac{t}{b}}}{1-e^{-\frac{\varepsilon}{b}}}R(H-t)\,dt \\ &+ \int_{\varepsilon}^{H} A_y e^{-\frac{t}{\tau_{O3}}}\,R(H-t)\,dt \qquad (21)\\ &= \sum_{j=1}^{2}\frac{A_y c_j}{d_j(1-e^{-\frac{\varepsilon}{b}})}\int_0^{\varepsilon}(1-e^{-\frac{t}{b}})\,e^{-\frac{H-t}{d_j}}\,dt \\ &+ \sum_{j=1}^{2}\frac{A_y c_j}{d_j}\int_{\varepsilon}^{H} e^{-\frac{t}{\tau_{O3}}}\,e^{-\frac{H-t}{d_j}}\,dt \qquad (22)\end{aligned}$$

Table 1: Error in option 1 vs option 2 for AGWP and AGTP for $H = 20$ and $b = 0.025\varepsilon$.

ε	AGWP	AGTP
1/12	0.08 %	−1.3 %
2/12	0.31 %	−2.1 %
3/12	0.57 %	−2.6 %

$$\begin{aligned}&= \sum_{j=1}^{2}\frac{A_y c_j}{d_j(1-e^{-\frac{\varepsilon}{b}})}\cdot \\ &\qquad \int_0^{\varepsilon} e^{-\frac{H-t}{d_j}} - e^{-t(\frac{1}{b}-\frac{1}{d_j})-\frac{H}{d_j}}\,dt \\ &+ \sum_{j=1}^{2}\frac{A_y c_j}{d_j}\int_{\varepsilon}^{H} e^{-t(\frac{1}{\tau_{O3}}-\frac{1}{d_j})-\frac{H}{d_j}}\,dt \\ &= \sum_{j=1}^{2}\frac{A_y c_j}{d_j(1-e^{-\frac{\varepsilon}{b}})}\left|d_j e^{-\frac{H-t}{d_j}}\right. \\ &\qquad \left.-\frac{-1}{\frac{1}{b}-\frac{1}{d_j}}e^{-t(\frac{1}{b}-\frac{1}{d_j})-\frac{H}{d_j}}\right|_0^{\varepsilon} \\ &+ \sum_{j=1}^{2}\frac{A_y c_j}{d_j}\left(\frac{-1}{\frac{1}{\tau_{O3}}-\frac{1}{d_j}}\right)\cdot \\ &\qquad \left|e^{-t(\frac{1}{\tau_{O3}}-\frac{1}{d_j})-\frac{H}{d_j}}\right|_{\varepsilon}^{H} \\ &= \sum_{j=1}^{2}\frac{A_y\,c_j}{1-e^{-\frac{\varepsilon}{b}}}\left[e^{-\frac{H-\varepsilon}{d_j}}-e^{-\frac{H}{d_j}}\right. \\ &\qquad \left.+\frac{b}{b-d_j}\left(e^{-\varepsilon(\frac{1}{b}-\frac{1}{d_j})-\frac{H}{d_j}}-e^{-\frac{H}{d_j}}\right)\right] \\ &+ \sum_{j=1}^{2}\frac{A_y\,\tau_{O3}\,c_j}{\tau_{O3}-d_j}\cdot \\ &\qquad \left(e^{-\frac{H}{\tau_{O3}}}-e^{-\varepsilon(\frac{1}{\tau_{O3}}-\frac{1}{d_j})-\frac{H}{d_j}}\right)\end{aligned}$$

The error in option 1 compared to option 2 varies for the choice of ε, shown in Table 1 for time horizon $H = 20$. $\overline{F_{O3}}$ is a factor in both A_{O3} and A_y, so its value does not matter for the percent error.

Withing 1–3 months the error in AGTP and AGWP is between 1–3%, which is small enough for our use.

1.3 H_2O

The response lifetime for H_2O is short, assumed to be 0.05 years, giving the same assumption as for AIC:

$$A_{H2O} = \frac{\overline{F_{H2O}}}{\tau_{H2O}\left(1-e^{-\frac{t}{\tau_{H2O}}}\right)} \approx \frac{\overline{F_{H2O}}}{\tau_{H2O}} \qquad (23)$$

Having the pulse and its decay rate, we have the forcing as a function of time:

$$F_{H2O}(t) = A_{H2O}\,e^{\left(-\frac{t}{\tau_{H2O}}\right)} \qquad (24)$$

and we calculate AGWP using Eqn. (1):

$$AGWP_{H2O} = \int_0^H F_{H2O}(t)\,dt$$

$$= \quad A_{H2O}\,\tau_{H2O}\left(1-e^{-\frac{H}{\tau_{H2O}}}\right) \quad (25)$$

And AGTP:

$$AGTP = \int_0^H F_{H2O}(t)\,R(H-t)\,dt \quad (26)$$

where R is the usual response function in Eqn. (3). Solving Eqn. (26) using Eqn. (24) and Eqn. (3), we get:

$$AGTP_{H2O} = \sum_{j=1}^{2} \frac{A_{H2O}\,\tau_{H2O}\,c_j}{\tau_{H2O}-d_j}\left(e^{-\frac{H}{\tau_{H2O}}} - e^{-\frac{H}{d_j}}\right) \quad (27)$$

1.4 CH_4

CH_4 has a response time of about 12 years, hence differing substantially from the previous components. An emission of NO_x produces a negative perturbation in CH_4 through increase in OH, and this perturbation reaches its minimum after a time H_0. From that point, the perturbation decays according to the response lifetime. From the model we have the integrated forcing up to H_0 and the minimum RF (F_m) at H_0.

For simplicity, we approximate the response from $t = 0$ to $t = H_0$ as a linear function, and after $t = H_0$ as an exponential decay:

$$\begin{aligned} F_{CH4}(t) &= \frac{t}{H_0}F_m \qquad \text{for } 0 \le t \le H_0 \quad (28)\\ F_{CH4}(t) &= F_m\,e^{\frac{-(t-H_0)}{\tau_{CH4}}} \qquad \text{for } H_0 < t \end{aligned}$$

This can then be integrated to find AGWP and AGTP (in the following we simplify the notation by writing τ for τ_{CH4}):

$$\begin{aligned} AGWP_{CH4} &= \int_0^H F_{CH4}(t)\,dt \quad (29)\\ &= \int_0^{H_0} \frac{t}{H_0}F_m\,dt \\ &\quad + \int_{H_0}^{H} F_m\,e^{\frac{-(t-H_0)}{\tau}}\,dt \\ &= \frac{H_0}{2}F_m \\ &\quad + \tau\,F_m\left(1-e^{\frac{-(H-H_0)}{\tau}}\right) \end{aligned}$$

$$\begin{aligned} AGTP_{CH4} &= \int_0^H F_{CH4}(t)\,R(H-t)\,dt \quad (30)\\ &= \int_0^{H_0} \frac{t}{H_0}F_m\,R(H-t)\,dt \\ &\quad + \int_{H_0}^{H} F_m\,e^{\frac{-(t-H_0)}{\tau}}\,R(H-t)\,dt \end{aligned}$$

and by inserting R, we get after re-arranging the integration and sums:

$$\begin{aligned} AGTP_{CH4} &= \sum_{j=1}^{2} \frac{c_j}{d_j}\frac{F_m}{H_0}\int_0^{H_0} te^{\frac{-(H-t)}{d_j}}\,dt \\ &\quad + \sum_{j=1}^{2} \frac{c_j}{d_j}F_m \int_{H_0}^{H} e^{-t(\frac{1}{\tau}-\frac{1}{d_j})+\frac{H_0}{\tau}-\frac{H}{d_j}}\,dt \end{aligned}$$

followed by partial integration of the first term and regular integration of the second term:

$$\begin{aligned} AGTP_{CH4} &= \sum_{j=1}^{2} \frac{c_j\,F_m}{d_j\,H_0}\cdot \\ &\quad \left| d_j\,t\,e^{\frac{-(H-t)}{d_j}} - d_j^2\,e^{\frac{-(H-t)}{d_j}} \right|_0^{H_0} \\ &\quad + \sum_{j=1}^{2} \frac{c_j\,F_m}{d_j}\frac{\tau\,d_j}{\tau-d_j}\cdot \\ &\quad \left| e^{-t(\frac{1}{\tau}-\frac{1}{d_j})+\frac{H_0}{\tau}-\frac{H}{d_j}} \right|_{H_0}^{H} \\ &= \sum_{j=1}^{2} \frac{c_j\,F_m}{H_0}\cdot \\ &\quad \left((H_0-d_j)\,e^{\frac{-(H-H_0)}{d_j}} + d_j\,e^{\frac{-H}{d_j}}\right) \\ &\quad + \sum_{j=1}^{2} \frac{c_j\,F_m\,\tau}{\tau-d_j}\cdot \\ &\quad \left(e^{\frac{-(H-H_0)}{\tau}} - e^{\frac{-(H-H_0)}{d_j}}\right) \end{aligned}$$

In this work, we assume that the $H_0 = 1$ year.

1.5 PMO

For PMO we assume $F_{PMO} = 0.29F_{CH4}$, hence we get:

$$\begin{aligned} AGWP_{PMO} &= 0.29\,AGWP_{CH4} \quad (31)\\ AGTP_{PMO} &= 0.29\,AGTP_{CH4} \quad (32) \end{aligned}$$

1.6 CO_2

CO_2 has a long lifetime, with specific forcing of $A_{CO2} = 1.82\cdot 10^{-15}\,\mathrm{Wm^{-2}kg(CO_2)^{-1}}$. With the assumption of 3.16 kg(CO_2) per kg(fuel), we get specific forcing of $A_{CO2} = 5.7512\cdot 10^{-15}\,\mathrm{Wm^{-2}kg(fuel)^{-1}}$. The time evolution of the response is given in Eqn. (A1) in F2010:

$$F_{CO2}(t) = A_{CO2}\left(a_0 + \sum_{i=1}^{3} a_i\,e^{-\frac{t}{\alpha_i}}\right) \quad (33)$$

with the parameters

$$\begin{aligned} a_0 &= 0.217\\ a_1 &= 0.259\\ a_2 &= 0.338\\ a_3 &= 0.186\\ \alpha_1 &= 172.9\\ \alpha_2 &= 18.51\\ \alpha_3 &= 1.186 \end{aligned}$$

Integrating Eqn. (33) from $t = 0$ to $t = H$, we get AGWP:

$$
\begin{aligned}
AGWP_{CO2} &= F_{CO2} \sum_{i=0}^{3} d_i \qquad (34) \\
d_0 &= a_0\, H \\
d_1 &= a_1\, (1 - e^{-\frac{H}{\alpha_1}}) \\
d_2 &= a_2\, (1 - e^{-\frac{H}{\alpha_2}}) \\
d_3 &= a_3\, (1 - e^{-\frac{H}{\alpha_3}})
\end{aligned}
$$

AGTP is found by integrating Eqn. (2) using Eqn. (3) and Eqn. (33), which yields Eqn. (A3) in F2010:

$$
\begin{aligned}
AGTP_{CO2} &= F_{CO2} \left\{ \sum_{j=1}^{2} a_o\, c_j \left(1 - e^{-\frac{H}{d_j}}\right) \right. \qquad (35) \\
&\left. + \sum_{i=1}^{3} \sum_{j=1}^{2} \frac{a_i\, \alpha_i c_j}{\alpha_i - d_j} \left(e^{-\frac{H}{\alpha_i}} - e^{-\frac{H}{d_j}}\right) \right\}
\end{aligned}
$$

References

Fuglestvedt, J. S., Shine, K. P., Berntsen, T., Cook, J., Lee, D. S., Stenke, A., Skeie, R. B., Velders, G. J. M., and Waitz, I. A.: Transport impacts on atmosphere and climate: Metrics, Atm. Env., 44, 4648–4677, doi:10.1016/j.atmosenv.2009.04.044, 2010.