CLIMATE CHANGE
27/2024

Final report

Software for a simplified estimation of CO_2 equivalents of individual flights

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Abstract: Software for a simplified estimation of CO_2 equivalents of individual flights

In order to achieve a reduction in non-CO_2 effects, the European Parliament (EP) voted on June 8, 2022 to expand the scope of the EU Emission Trading System (EU ETS) (EP, 2022) to non-CO_2 effects. In December 2022 the European Council, the European Commission (EC) and the EP reached an agreement on the revision of the EU ETS. According to the agreement, non-CO_2 effects can no longer be ignored and the EC should set up a monitoring, reporting and verification (MRV) scheme for non-CO2 aviation emissions from 2025, as a first step for the full integration of non-CO2 effects into the EU ETS. This project focuses on the development and testing of such an MRV system. For this purpose, non-CO2 effects are integrated according to the principle of equivalent CO_2 emissions (CO2e). Since several CO2e calculation methods are in principle available, the selection process involves a trade-off between the level of atmospheric uncertainties, the level of climate mitigation incentives, and the resulting effort of MRV activities (see Section 1.2).

The present report is about the development of an application for a simplified estimate of CO_2 equivalents per flights. The simplified calculation method should estimate non-CO_2 climate effects of air traffic as precisely as possible, without detail information of the actual flight route, actual fuel burn and the current weather situation. For this purpose, we evaluate a data set containing a global set of detailed flight trajectories, flight emissions and climate responses (see Section 2.1). Based on the data set regression formulas for fuel consumption, NO_x emissions (see Section 2.3) and climate responses (see Section 3) are generated. A user manual of the tool is described in section 4. This simplified estimate of CO_2 equivalents is not intended for the use in an emission trading system, but could serve for plausibility checks or as a backup, if airlines are not able to provide the needed data.

Kurzbeschreibung: Software zur vereinfachten Abschätzung von CO_2-Äquivalenten einzelner Flüge

Mit dem Ziel, die Klimawirkung des Luftverkehrs zu reduzieren, votierte das Europäische Parlament (EP) am 8. Juni 2022 dafür, das EU-Emissionshandelssystem (EU ETS) um Nicht-CO_2-Effekte zu erweitern (EP, 2022). Im Dezember 2022 einigten sich der Europäische Rat, die Europäische Kommission (KOM) und das EP auf eine entsprechende Änderung des EU ETS. Gemäß des Gesetzesänderungsbeschlusses dürfen Nicht-CO_2-Effekten Effekte nicht länger ignoriert werden und sollen, als erster Schritt zur vollständigen Integration in das EU-ETS, ab 2025 durch ein von der KOM entworfenes Überwachungs-, Berichterstattungs- und Verifizierungssystem (MRV) erfasst werden. Dieses Projekt behandelt die Entwicklung und Erprobung eines solchen Systems. Die Nicht-CO_2-Effekte werden dabei nach dem Prinzip der CO_2-Äquivalente (CO2e) erfasst. Da verschiedene Ansätze zur Berechnung von CO2e zur Verfügung stehen, muss bei der Wahl der Berechnungsmethode eine Abwägung zwischen möglichst geringen atmosphärischen Unsicherheiten, möglichst hohen Klimaschutzanreizen und ein möglichst geringer Aufwand für MRV-Aktivitäten gefunden werden (siehe Abschnitt 1.2).

Der vorliegende Bericht befasst sich mit der Entwicklung einer Anwendung zur vereinfachten Abschätzung von CO_2-Äquivalenten pro Flug. Die vereinfachte Berechnungsmethode soll Nicht-CO_2-Klimaeffekte des Flugverkehrs möglichst genau abschätzen, ohne auf Detailinformationen über die tatsächliche Flugroute, tatsächlichen Treibstoffverbräuchen und aktuelle Wettersituationen zurückgreifen zu müssen. Zu diesem Zweck werten wir einen globalen Datensatz von detaillierter Flugtrajektorien aus, der die dabei ausgestoßenen Flugemissionen und Klimareaktionen enthält (siehe Abschnitt 2.1). Auf Basis dieses Datensatzes werden Regressionsformeln für Treibstoffverbrauch, NO_x-Emissionen (siehe Abschnitt 2.3) und Klimareaktionen (siehe Abschnitt 3) erstellt. Ein Benutzerhandbuch für das Tool wird in Abschnitt 4 beschrieben. Diese vereinfachte Schätzung der CO_2-Äquivalente ist nicht für die Verwendung in einem Emissionshandelssystem gedacht, sondern kann zur Plausibilitätsprüfung oder als Backup dienen, falls die Fluggesellschaften nicht in der Lage sind, die erforderlichen Daten zu liefern.

Table of content

List of figures

List of tables

List of abbreviations

$AGWP_{100}$	Absolute global warming potential over 100 years
ATR_{100}	Average temperature response over 100 years
CiC	Contrail induced cloudiness
CH_4	Methane
CO_2	Carbon dioxide
CO2e	Carbon dioxide equivalent
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
EC	European Commission
EU-ETS	EU Emissions Trading System
GHG	Greenhouse gas
H_2O	Water vapor
ICAO	International Civil Aviation Organization
MBM	Market-based measure
MRV	Monitoring, reporting and verification
NO_x	Nitrogen oxides
O_3	Ozone
RF	Radiative forcing
SAC	Schmidt-Appleman Criterion
SAF	Sustainable Aviation Fuel

1 Introduction

1.1 Short overview of climate effects of aviation and possible mitigation approaches

The climate change gets more and more noticeable. Over the last decades, global aviation in terms of revenue passenger kilometers has doubled every 15 years and is expected to grow further (e.g., ICAO, 2013a). As aviation is one of the fastest growing sectors, the share in global CO_2 emission could rise from currently about 2 up to even 22% in 2050 (Cames et al., 2015).

Beside CO_2 emissions, also non-CO_2 emissions contributes to aviation induced climate change. Especially the impact of contrail cirrus and the effect of NO_x emissions on the concentration of ozone increases the climate impact of aviation. The impact of non-CO_2 effects of the historical emissions of aviation caused about two third of the total aviation impact (Lee et al., 2021).

There are different options to mitigate the climate impact of aviation. Beside reducing the number of flights, the climate impact can be reduced by technical measures, alternative fuel or operational measures. Technical measures include reduction of specific fuel consumption, reduced weight and optimized aerodynamic. In addition, optimized aircraft design for flying in lower altitudes or a broader altitude band could reduce offsets of flying climate optimized. The climate impact can also be reduced by using alternative fuels like sustainable aviation fuel (SAF) or liquid hydrogen. This does not only reduce the impact of CO_2 (as it is climate neutral if the fuel is produced with renewable energy), but has also an impact on non-CO_2 effects, e.g. contrails. Efficient flight guidance can reduce the fuel consumption and the impact on climate. As climate impact depends beside the emission strength also on emission location and time of emission, it is possible to reduce the climate impact if climate sensitive regions are avoided (climate optimized flights).

The climate mitigation of non-CO_2 effects often come along with an increase of cash operating costs. As operators of aircraft have little incentives to pay these additional costs voluntarily, incentives for reducing climate impacts of non-CO_2 effects are necessary. Therefore, including also non-CO_2 effects in emission trading schemes or marked based measures (MBM) could be a significant contribution to the agreed climate goals of Paris.

1.2 Options for estimating CO_2 equivalents of individual flights

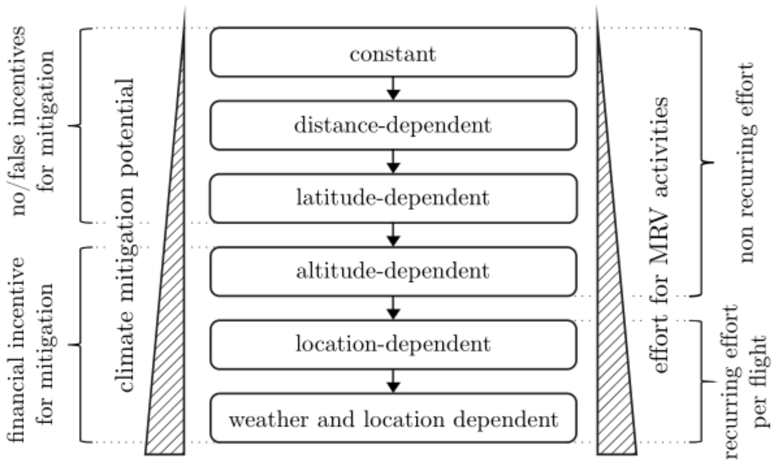
Carbon dioxide equivalents (CO2e or CO2eq or CO2-e) are a common metric for unitizing the climate impact of various climate agents. Since the climate impact of CO_2 is well understood (due to its independence of emission source and location) and one of the major anthropogenic greenhouse gasses, it is reasonable to express the impacts of non-CO_2 effects in relation to the impacts of one kg of CO_2. For a given type and amount of a climate agent *i*, resulting CO2e cause the same climate response (e.g. RF or ΔT) over a specific time horizon (e.g. 20, 50 or 100 years) as CO_2:

$$\mathrm{CO2e}_{\mathrm{agent}\ i} = \frac{\mathrm{Climate\ Impact}_{\mathrm{agent}\ i}}{\mathrm{Climate\ Impact}_{1\ \mathrm{kg\ CO2}}}$$

$$\mathrm{CO2e}_{\mathrm{total}} = \mathrm{CO}_2 + \sum_i \mathrm{CO2e}_{\mathrm{agent}\ i}$$

In principle, there are several CO2e calculation methods available (see Figure 1) that are designed for different applications and differ, among other things, in the accuracy of the climate assessment. As a general rule, CO_2 equivalents should be easily calculable, predictable and transparent. If CO2e are used for the compensation market or emissions trading, the calculation method must create incentives to actually reduce non-CO_2 effects. In order to avoid misguiding incentives at least the altitude dependency of non-CO_2 effects has to be considered in the CO2e calculation method (Faber et al., 2008; Niklaß et al., 2020; Scheelhaase et al., 2016). This requires at least detailed information about the flown aircraft trajectory (altitude profile) of each flight. However, the query of flight data is an elaborate process that does not have to be carried out for ecological footprint assessments of single flights. Instead, much simpler CO2e calculation methods can be used here.

Figure 1: Mitigation benefit and MRV effort of different CO2e calculation methods (adapted from Niklaß et al. 2020, p.43).



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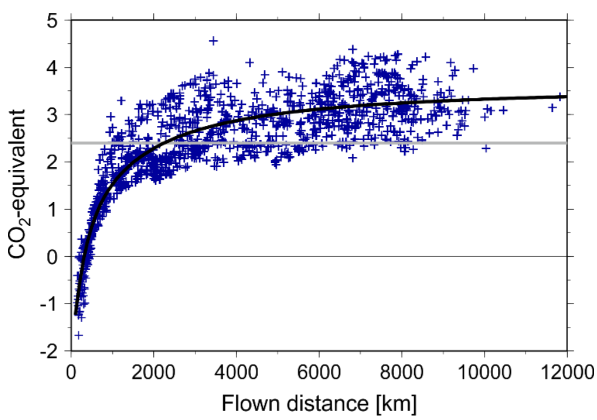
The simplest options are constant CO2e factors, such as the Radiative Forcing Index (RFI), as well as distance-dependent ones. The accuracy of these simple factors was investigated, for example, by Dahlmann et al. (2021), who analysed the climate impact of one typical long-haul aircraft type of A330-200 aircraft for more than 1000 international city pairs. Results of this study are shown in Figure 2, which plots calculated CO_2 equivalent factors from the climate response model *Airclim* (blue crosses) (Dahlmann et al., 2016) against simplified CO2e estimates (a constant factor of 2.4 is shown as a gray line).

Figure 2: Climate impact in CO_2 equivalent factors of total non-CO_2 emissions in dependency of flight distances (blue crosses) as well as the constant factor (gray line) and the parametric values analyzed with the function flight distance dependency (black line). To obtain total CO2e values the impact of CO_2 (per definition equal 1) has to be added.



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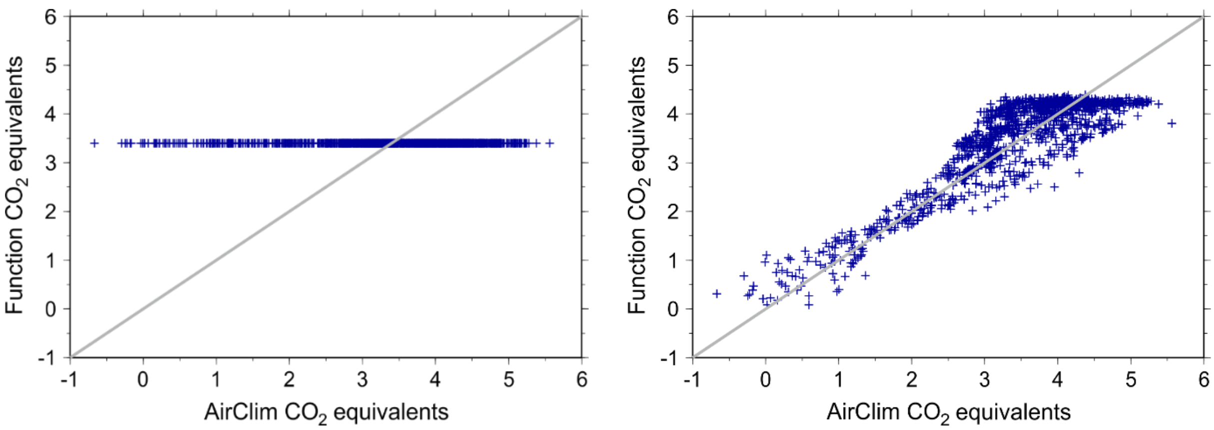
In general, we see an increase of CO2e factors because increasing flight distances also increases the average flight altitude. This increase in total CO2e values becomes less significant for flight distances longer than 4000 km, as average flight altitudes hardly changes on long-haul flights. With the total CO2e dependence on distance showing a large change for small distances but a smaller one for large distances, Dahlmann et al. (2021) fitted arc tangent functions to the results (black lines in Figure 2) that obey the pattern

$$\mathrm{CO2e}_{\mathrm{agent}}(D) = a_0 + a_1 \cdot \arctan(a_2 \cdot d)$$

While the constant factors show large deviations from the calculated CO2e values, there is much higher agreement with distance-dependent factors. This is also illustrated in Figure 3, showing the correlation between the CO2e factors calculated with *AirClim* and simplified estimate based on constant (left) and distance dependent (right) CO2e factors. Gray lines represent perfect agreements.

Figure 3: Correlation between CO_2 equivalent (CO2e) factors calculated with *AirClim* and simplified estimate based on constant (left) and distance dependent (right) CO2e factors. To obtain total CO2e values the impact of CO_2 (per definition equal 1) has to be added.



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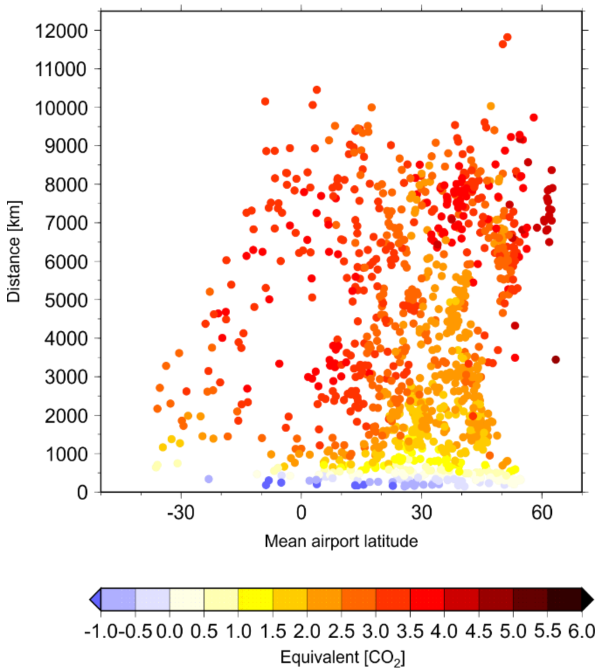
For a constant factor of 3.4, only very few missions are correctly represented. The specific climate impact is underestimated by up to about 40% (mean square error is about 1.18) or shows even a wrong sign compared to the *AirClim* results. By applying a flight distance dependent factor, 95% of the estimates lie within a ±20% range, which reduces the root mean square error to about 0.24.

Integrating the latitudinal dependency in addition to the distance dependency in the calculation formulas further increases the accuracy of the results. Such an approach was carried out by Dahlmann et al. (2021), who defined 4th order polynomial equations:

$$\mathrm{CO2e}_{\mathrm{agent}}(L, D) = \left(a_{\mathrm{agent},0}L^4 + a_{\mathrm{agent},1}L^3 + a_{\mathrm{agent},2}L^2 + a_{\mathrm{agent},3}L + a_{\mathrm{agent},4}\right)\left(a_{\mathrm{agent},5}D + a_{\mathrm{agent},6}\right)$$

where L is the mean-latitude in deg North between origin and destination airport, $\underline{\underline{D}}$ is the flown distance in 1000 km, and $a_{\mathrm{agent},0}$ to $a_{\mathrm{agent},6}$ are polynomial coefficients. This further reduces the mean square error to about 0.19. Calculated CO2e factors in dependency of the flown distances and mean latitude are show in Figure 4.

Figure 4: CO_2 equivalent factors of all non-CO_2 effects in dependence of mean latitude and flight distance. To obtain total CO2e values the impact of CO_2 (per definition equal 1) has to be added.



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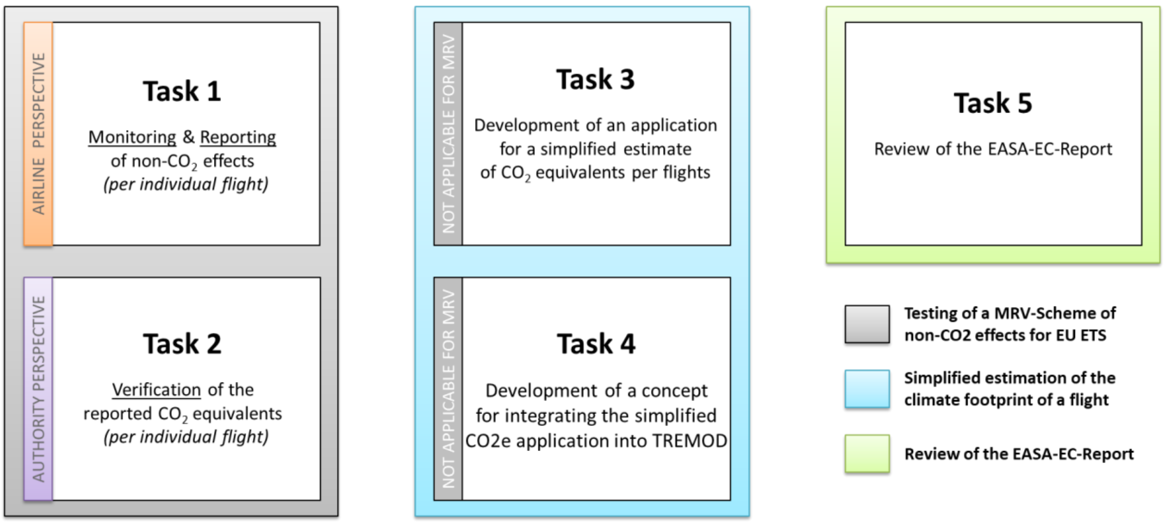
CO2e regression formulas for aircraft types other than the A330 are not available. For larger route networks and different aircraft categories, clusters (e.g. for different climate zones or different distance categories) might also help to further increase the accuracy of CO2e regressions formulas.

1.3 Integration into the Project

In this project on behalf of the German Environment Agency (UBA), three out of five work packages focus on the calculation of non-CO_2 climate effects (see Figure 5). The present report is about the development of an application for a simplified estimate of CO_2 equivalents per flights (task 3).

Figure 5: Overview of current project activities



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The simplified calculation method should estimate non-CO_2 climate effects of air traffic as precisely as possible, without detail information of the actual flight route, the amount of emissions and the current weather situation. For this purpose, we evaluate a data set containing a global set of detailed flight trajectories, flight emissions and climate responses (see Section 2.1). Based on the data set regression formulas for fuel consumption, NOx emissions (see Section 2.3) and climate responses (see Section 3) are generated. A user manual of the tool is described in section 4. This simplified estimate of CO2 equivalents is not intended for use in an emissions trading system but could be applied for plausibility checks or as a backup when airlines are unable to provide the required data

In work package 1 and 2, we take the perspective of an aircraft operator and a government agency to test all steps for monitoring, reporting, and verification (MRV) of CO_2 equivalents (see Plohr et al., 2022; Niklaß et al., 2023). Calculated CO2e values for all three approaches are compared in work package 2 (see Niklaß et al., 2023).

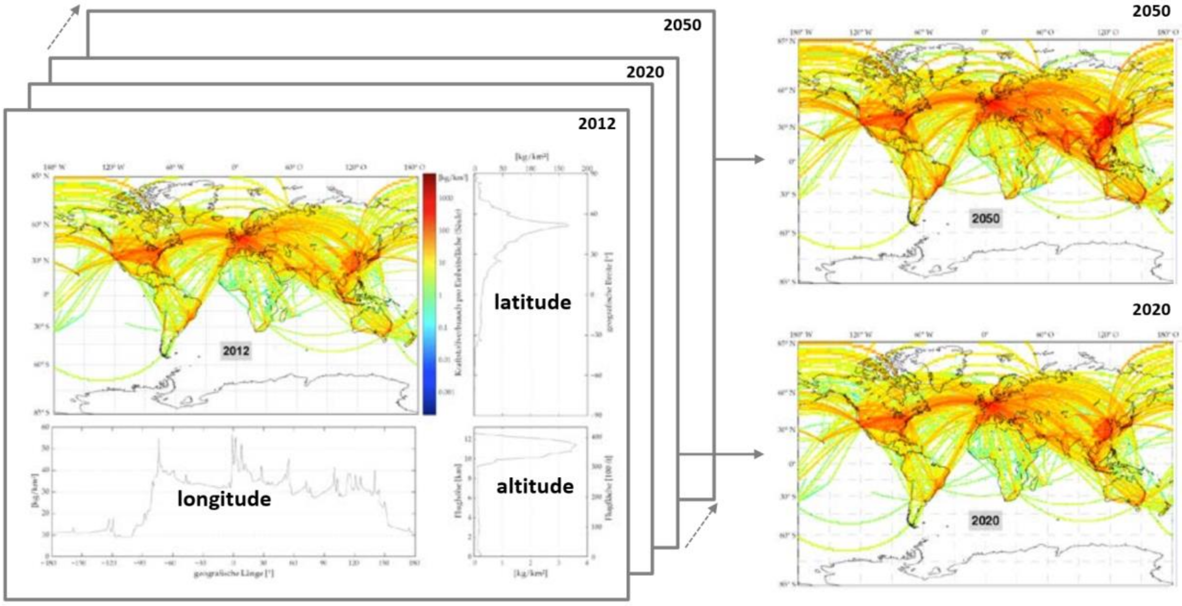
2 Data Basis

As a basis for the derivation of regression formulas that allow for the determination of CO_2 equivalent emissions (see chapter 3), data from the former DLR internal project WeCare (Utilizing Weather information for Climate efficient and ecoefficient future aviation) was used. The project ran from 2013 to 2017 an addressed both an improvement of the understanding of aviation-influenced atmospheric processes and an assessment of different mitigation options. An essential output of the project was a new set of emission inventories for global aviation (Grewe et al., 2017). These datasets constitute the basis for this work and are described in more detail in the following sections.

2.1 Global emission inventories and climate responses of the DLR project WeCare

One of the objectives of the WeCare project was to create new global aviation emission inventories to be used to assess the climate impact of aviation. These inventories were developed following a four-layer approach implemented in the AIRCAST methodology (Ghosh et al., 2016), starting from an origin-destination passenger demand network that was built-up from exogenous socio-economic scenarios, via the passenger routes network (sequence of flight segments, a passenger actually travelled from origin to destination) to an aircraft movements network, which assigns aircraft categories to the resulting flight routes and provides flight frequency information. The final step constitutes a simulation of trajectories based on the aircraft movements obtained from the Aircraft Movements Network layer using the Global Air Traffic Emissions Distribution Laboratory (GRIDLAB) developed by DLR (Linke, 2016). Each mission defined by departure and arrival cities, aircraft type and load factor was simulated under typical operational conditions, resulting in a network of flight trajectories. For this purpose, DLR's Trajectory Calculation Module (TCM) (Lührs et al., 2014) was used that applies simplified equations of motion known as the Total Energy Model. Based on the aircraft's engine state (e.g. thrust, fuel flow) the engine emission distribution of NO_x, CO and HC species along the trajectory was determined applying the Boeing Fuel Flow Method 2 (DuBois et al., 2006). The amount of CO_2 and H_2O was calculated assuming a linear relationship to the fuel burn. The emission distributions of all flights were mapped into a geographical grid resulting in 3D inventories. These were the essential input for the climate impact assessment tool *AirClim* (Dahlmann et al., 2016), which determines concentration changes of different radiative forcing agents (CO_2, H_2O, O_3) as well as aviation-induced cloudiness. Based on that, various climate metrics for the given emission scenario were calculated. In WeCare, using the approach mentioned above, emission inventories and the corresponding climate impact were calculated for the years 2015 to 2050 in 5-year steps, while the forecast was based on the reference year 2012. The resulting flight plan of the base year consisted of 47.057 airport pairs and approximately 31 million flights. As it was found that aircraft with more than 100 seats contribute to about 95% of the globally available seat kilometres (ASK), only aircraft larger than 100 seats were covered by the study to reduce complexity and ensure model availability. Therefore, five different aircraft size categories (based on the number of seats) were considered in the inventories (101-151 seats; 152-201 seats; 202-251 seats; 252-301 seats; 302-600 seats) and each size category was modelled using one representative aircraft type (plus one backup aircraft type). The representative aircraft type was selected such that it contributes to a significant share of the respective size category. Respective engine emission characteristics were taken from the ICAO Aircraft Engine Emissions Databank.

Figure 6: Aggregated global air traffic emission inventories until 2050 from the WeCare project



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2.2 Processing of WeCare data

From the WeCare project only aggregated flight and emission inventories were available. The determination of regression formulas that can be applied to individual flights requires a disaggregation of the WeCare dataset. Therefore, for the entire flight inventory from WeCare emission distributions were calculated on a per-flight basis following the above described methodology. The resulting single trajectory inventories were then processed with the climate assessment tool *AirClim*, to obtain the climate impact metrics per species for each flight in the flight plan. The results were stored in an Access database to allow for an efficient handling of the resulting data including data queries, sorting and filtering. In the data structure for each flight characterized by origin and destination airport as well as aircraft size category, the resulting amounts of engine emissions were stored together with the climate impact per species. From that database the mathematical relationships were derived.

2.3 Derivation of fuel and NO_x functions

Using the access database, all flights of a seat category were selected. For each data set a regression formula is derived which approximates the burnt fuel (BF) and the emission index of NO_x (EI_{NO_x}) for a given flight distance (d). Fuel functions obey the pattern

$$\mathrm{BF} = a_0 + a_1 \cdot d + a_2 \cdot d^2$$

with the coefficients a as given in Table 1.

Table 1: Best fit solutions for fuel regression formulas

Seat Category	Max. Range (km)	a_0	a_1	a_2	R^2
101-151	6,000	632.36	2.5809	5.01E-05	1.000
152-201	7,000	629.27	2.5388	3.83E-05	0.999
202-251	13,000	997.62	4.6586	7.32E-05	0.999
252-301	13,450	3,770,.31	5.7234	3.77E-04	0.999
302-600	14,500	2,277.30	8.5406	2.38E-04	1.000

Derived EI_{NO_x} regression formulas vary for distances smaller and larger than 2000 km.

$$\text{EINOx} = \begin{cases} a_0 + a_1 \cdot \ln(d) & if\ d < 2000\ km \\ a_2 + a_3 \cdot d + a_4 \cdot d^2 + a_5 \cdot a^3 & if\ d \geq 2000\ km \end{cases}$$

Best fit solutions for EI_{NO_x} regression formulas are provided in Table 2.

Table 2: Best fit solutions for $EINO_x$ regression formulas

Seat Category	a_0	a_1	R^2	a_2	a_3	a_4	a_5	R^2
101-151	34.403	-2.667	0.868	17.478	-2.493E-03	5.232E-07	-3.660E-11	0.975
152-201	26.942	-2.135	0.881	13.163	-1.701E-03	3.251E-07	-2.050E-11	0.985
202-251	35.813	-3.007	0.923	14.742	-1.139E-03	1.534E-07	-6.290E-12	0.970
252-301	29.287	-2.221	0.930	13.428	-5.998E-04	6.578E-08	-2.374E-12	0.933
302-600	31.803	-2.488	0.971	13.992	-7.569E-04	9.646E-08	-3.375E-12	0.972

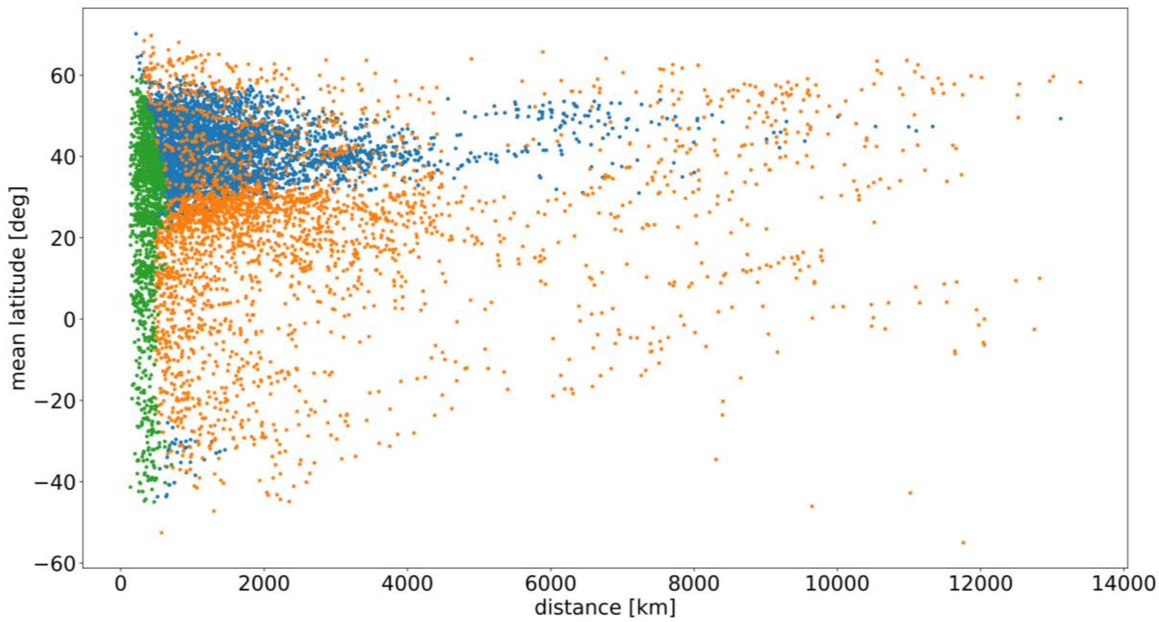
3 Clustering of climate response inventories and derivation of simple regression

This section describes the clustering of flight connection based on their climate effect components and the derivation of regression formulas, which allow for a quick determination of the climate effect of a flight for each of three detected clusters.
The analysis in this section is based on a set of 34790 flight connections (airport pairs) and uses the following quantities: flight distance along a great circle, mean latitude along the great circle, fuel use, NO_x emissions, and climate effect. The climate effect uses the average temperature response over 100 years (ATR100) as a metric, and is further divided into climate effect through different pathways (CO_2, H_2O, contrail cirrus, O_3, PMO, CH_4).
In the first step, the flight connections are clustered using the K-Means clustering algorithm. This clustering is based solely on the share of the six aforementioned components of the climate effect in the total climate effect:

$$\frac{\mathrm{ATR100_{CO_2}}}{\mathrm{ATR100_{tot}}}, \frac{\mathrm{ATR100_{H_2O}}}{\mathrm{ATR100_{tot}}}, \frac{\mathrm{ATR100_{CiC}}}{\mathrm{ATR100_{tot}}}, \frac{\mathrm{ATR100_{O_3}}}{\mathrm{ATR100_{tot}}}, \frac{\mathrm{ATR100_{PMO}}}{\mathrm{ATR100_{tot}}}, \frac{\mathrm{ATR100_{CH_4}}}{\mathrm{ATR100_{tot}}}$$

This ensures that connections in a given cluster have similar climate effect characteristics. The clustering is not directly dependent on proxy quantities to the climate effect, such as the emissions and the emission location. We use an implementation by scikit-learn (Pedregosa et al., 2011) and scale the input quantities to the standard normal distribution before clustering. We find a partition into three clusters to be most useful, as larger numbers of clusters lead to some clusters, whose distinctions do not have a clear physical interpretation.

Figure 7: Clustering of flight connections, as obtained by the K-Means clustering algorithm, shown in the latitude-distance space. Each color corresponds to one cluster.



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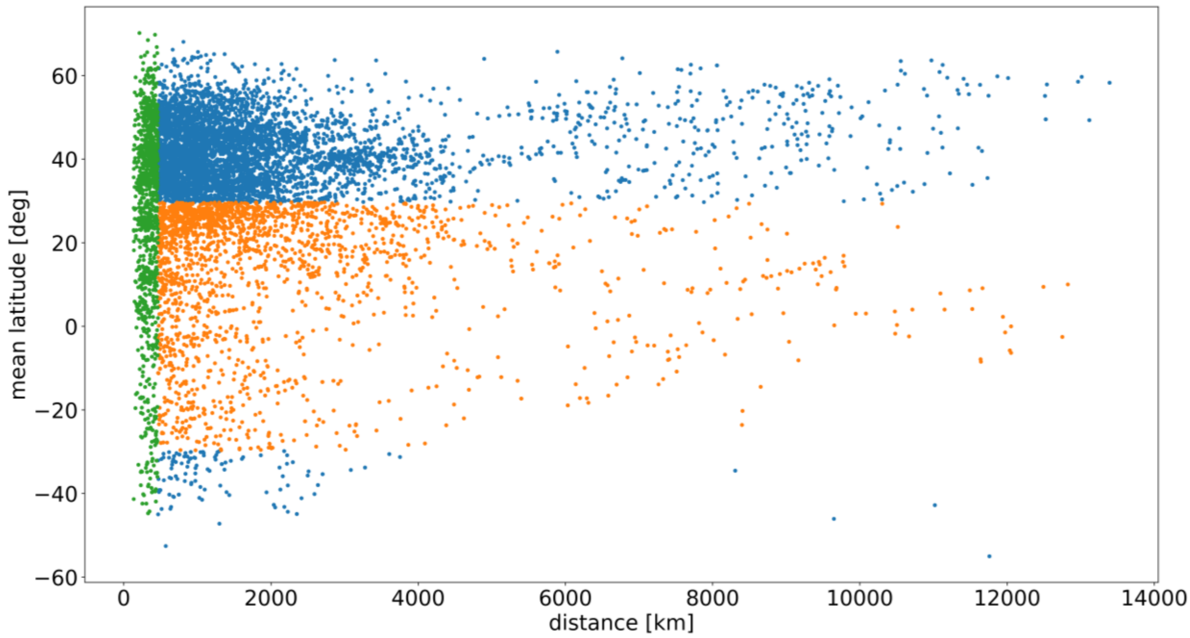
The resulting three clusters (Figure 7) have distinct characteristics. The short-flight cluster (green) has a negligible contribution of contrails to the climate effect, and a strong contribution of CO_2. Flight connections in this cluster often do not reach sufficient altitudes for contrail formation. The climate effect of the tropical cluster (orange) is dominated by contrails because contrails have a particularly large climate effect in the tropics. The mid-latitude cluster (blue) contains the remaining flight connections and has large climate effect contributions from NO_x and H_2O.

Figure 8: Three clusters of flight connections, delineated by simple thresholds, shown in the latitude-distance space. Each color corresponds to one cluster.



In the second step, simple thresholds are derived which separate the flight connections into three categories that approximate the found clusters. This is necessary to be able to categorize also new flight connections that are not contained in the data set used for this analysis. One threshold is a maximum distance for the short-flight cluster, and another threshold is the absolute mean latitude confining the tropical cluster. We choose the values for these thresholds in such a way that the amount of wrongly categorized flight connections is minimized. This leads to a threshold distance of 462.5 km below which connections are categorized as belonging to the short-flight cluster, and a threshold mean latitude of ±29.7° within which flight connections are categorized as belonging to the tropical cluster. All other flight connections are categorized into the mid-latitude cluster. This approximation wrongly categorizes 16.8% of flight connections (5859 flight connections). The resulting simplified clustering is shown in Figure 8.
In the third step, for each of the simplified clusters, a regression formula is derived which approximates the climate effect for a given flight. Following Dahlmann et al. (2021), the regression formulas obey the pattern

$$\mathrm{ATR100_{tot}} = c_{\mathrm{CO_2}} f + c_{\mathrm{NO_x}}(d, \bar{\phi}) e + c_{\mathrm{H_2O}}(d, \bar{\phi}) f + c_{\mathrm{CiC}}(d, \bar{\phi}) d,$$

where f is the fuel use, e are the NOx emissions, d is the flown distance, $\bar{\phi}$ is the mean latitude, $c_{\mathrm{CO_2}}$, $c_{\mathrm{NO_x}}$, $c_{\mathrm{H_2O}}$, and c_{CiC} are cluster-dependent regression formulas. These formulas are intended to fit the respective partial climate effects $\mathrm{ATR100_{CO_2}}$/f, $\mathrm{ATR100_{NO_x}}$/e, $\mathrm{ATR100_{H_2O}}$/f, and $\mathrm{ATR100_{CiC}}$/d, where $\mathrm{ATR100_{NO_x}} = \mathrm{ATR100_{O_3}} + \mathrm{ATR100_{PMO}} + \mathrm{ATR100_{CH_4}}$ is the combined climate effect of NOx emissions. The cluster-dependent regression formulas for CO_2 is fixed at cCO_2 = 8.145·10-11mKkg-1(fuel), because the same simple linear relationship is used during the computation of the ATR100 in *AirClim*, so that no fit is required.
The other cluster-dependent regression formulas are chosen based on the behavior of the respective values in latitude-distance space (Fig. 3-5) as

$$c_{\mathrm{NO_x}} = \left(a_{\mathrm{NO_x},s,0}d + a_{\mathrm{NO_x},s,1}\right)\left(a_{\mathrm{NO_x},s,2}\bar{\Phi}^4 + a_{\mathrm{NO_x},s,3}\bar{\Phi}^3 + a_{\mathrm{NO_x},s,4}\bar{\Phi}^2 + a_{\mathrm{NO_x},s,5}\bar{\Phi} + a_{\mathrm{NO_x},s,6}\right)$$

$$c_{\mathrm{H_2}O} = a_{\mathrm{H_2O},s,0}$$

$$c_{\mathrm{CiC}} = \left(a_{\mathrm{CiC},s,0}d^2 + a_{\mathrm{CiC},s,1}d + a_{\mathrm{CiC},s,2}\right)\bar{\Phi}^2$$

for the short-flight cluster,

$$c_{\mathrm{NO_x}} = a_{\mathrm{NO_x},m,0}\tan^{-1}\left(a_{\mathrm{NO_x},m,1}d\right) + a_{\mathrm{NO_x},m,2}d + a_{\mathrm{NO_x},m,3}$$

$$c_{\mathrm{H_2}O} = \left(a_{\mathrm{H_2O},m,0}\tan^{-1}\left(a_{\mathrm{H_2O},m,1}d\right)\right)\left(a_{\mathrm{H_2O},m,2}\bar{\Phi}^2 + a_{\mathrm{H_2O},m,3}\right)$$

$$c_{\mathrm{CiC}} = \left(a_{\mathrm{CiC},m,0}d^2 + a_{\mathrm{CiC},m,1}d + a_{\mathrm{CiC},m,2}\right)\left(a_{\mathrm{CiC},m,3}\bar{\Phi}^4 + a_{\mathrm{CiC},m,4}\bar{\Phi}^3 + a_{\mathrm{CiC},m,5}\bar{\Phi}^2 + a_{\mathrm{CiC},m,6}\bar{\Phi} + a_{\mathrm{CiC},m,7}\right)$$

for the mid-latitude cluster, and

$$c_{\mathrm{NO_x}} = \left(a_{\mathrm{NO_x},t,0}\tan^{-1}\left(a_{\mathrm{NO_x},t,1}d\right) + a_{\mathrm{NO_x},t,2}\right)\left(a_{\mathrm{NO_x},t,3}\bar{\Phi}^2 + a_{\mathrm{NO_x},t,4}\bar{\Phi} + a_{\mathrm{NO_x},t,5}\right)$$

$$c_{\mathrm{H_2}O} = \left(a_{\mathrm{H_2O},t,0}\tan^{-1}\left(a_{\mathrm{H_2O},t,1}d\right)\right)\left(a_{\mathrm{H_2O},t,2}\bar{\Phi}^2 + a_{\mathrm{H_2O},t,3}\right)$$

$$c_{\mathrm{CiC}} = \left(a_{\mathrm{CiC},t,0}\tan^{-1}\left(a_{\mathrm{CiC},t,1}d\right) + a_{\mathrm{CiC},t,2}d + a_{\mathrm{CiC},t,3}\right)\left(a_{\mathrm{CiC},t,4}\bar{\Phi}^4 + a_{\mathrm{CiC},t,5}\bar{\Phi}^2 + a_{\mathrm{CiC},t,6}\right)$$

for the tropical cluster, where the coefficients a are determined by a non-linear least-squares fit and are given by Table 1. The regression formulas can generally capture the trend, as can be seen by the fits (orange dots in Figure 9-Figure 11) and the mean absolute relative error, which is 9.4 % for the short-flight cluster, 16.1 % for the mid-latitude cluster, and 15.0 % for the tropical cluster. When combining results from the different clusters, this leads to a mean absolute relative error of 15.0 % and a root-mean-square error of 1.24 nK. The true model values obtained by *AirClim* are generally strongly correlated with the values obtained from the regression formulas (Figure 12).

Figure 9: **Climate metrics $\mathrm{ATR100}_{\mathrm{NO}_x}/e$ (top), $\mathrm{ATR100}_{\mathrm{H_2O}}/f$ (middle row), $\mathrm{ATR100}_{\mathrm{CiC}}/d$ (bottom) as a function of distance d (middle column), mean latitude $\overline{\phi}$ (right column), and both (left column) for the short-flight cluster. Blue dots denote the values obtained from *AirClim*, orange dots are fit results from the regression formula (Eq. 2)**

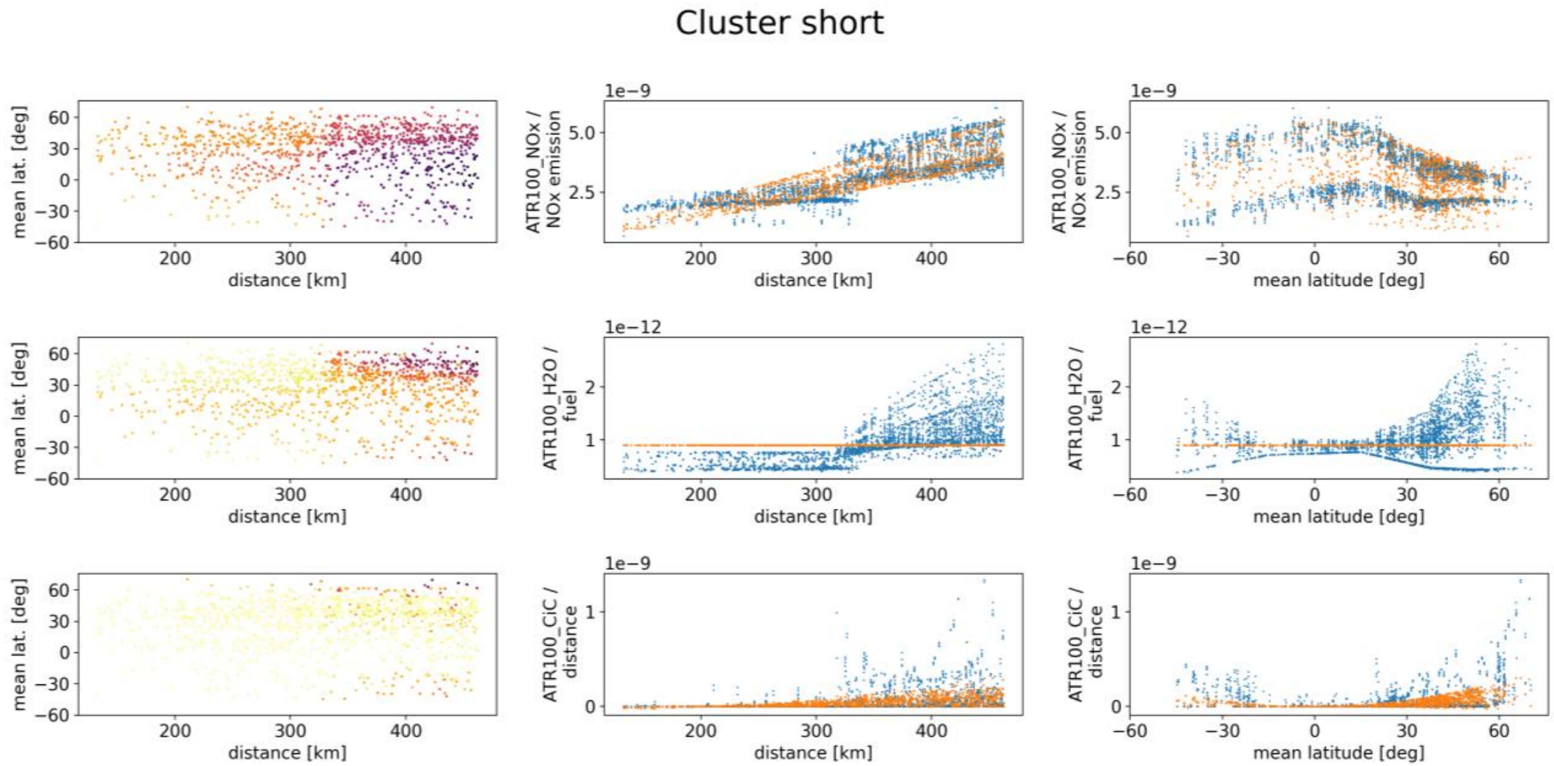


Figure 10: Same as Fig. 5, but for the mid-latitude cluster.

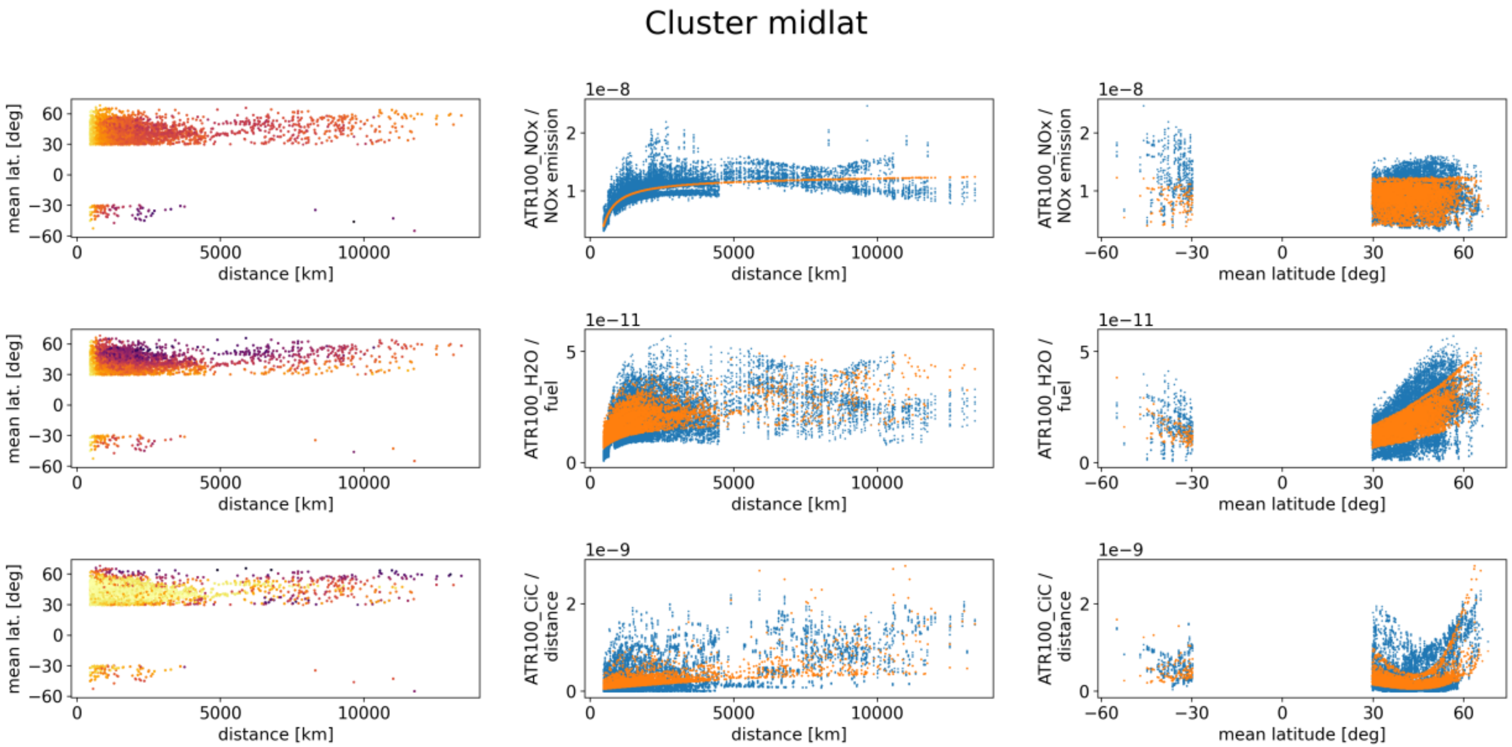


Figure 11: Same as Fig. 5, but for the tropical cluster.

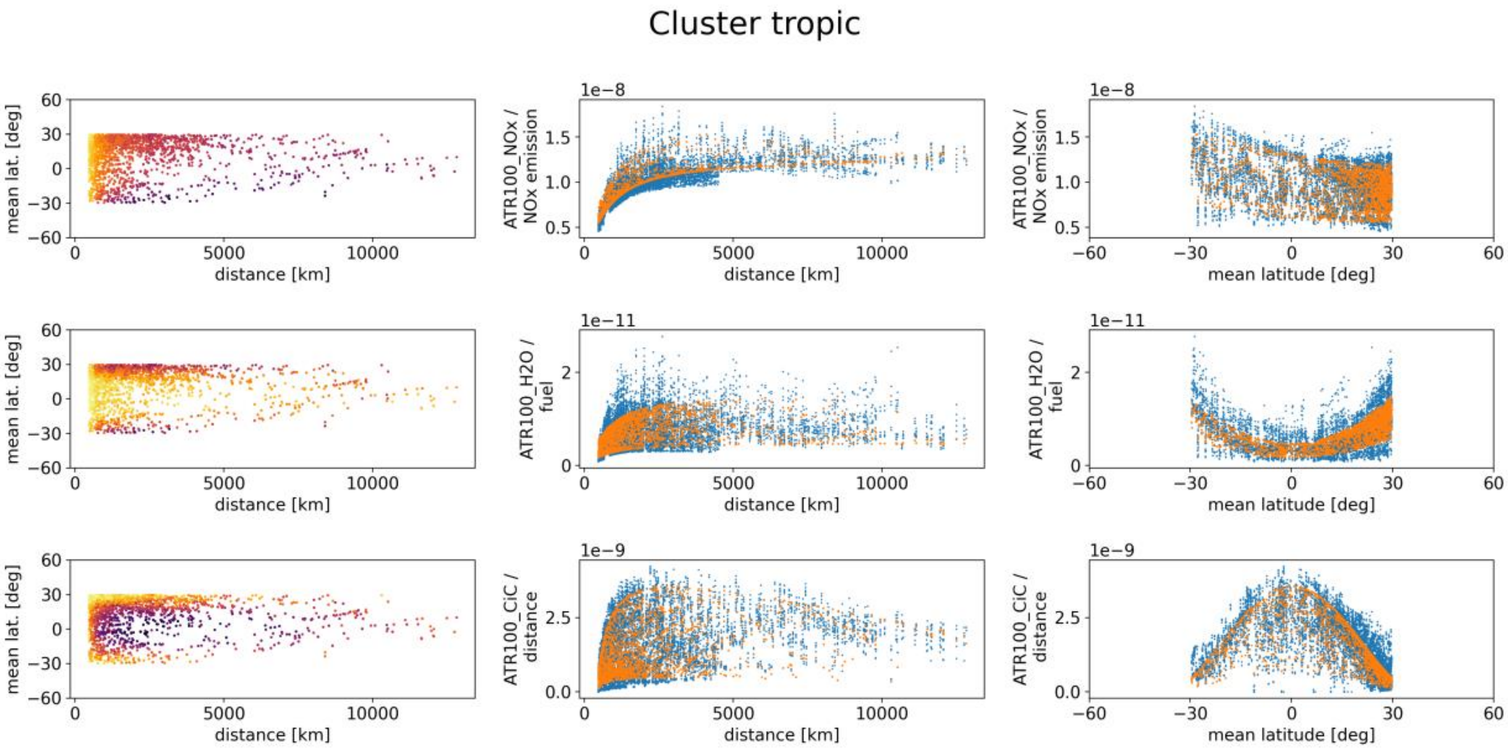
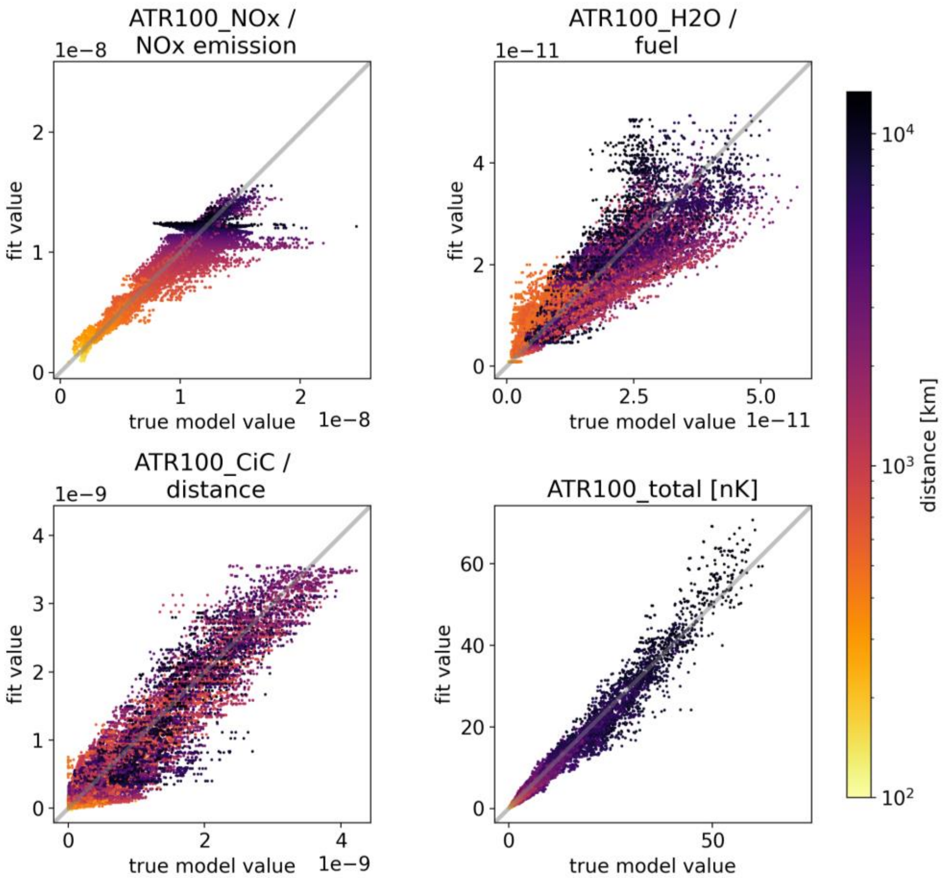


Figure 12: Correlation contrasting the true model values of quantities $ATR100_{NO_x}/e$, $ATR100_{H_2O}/f$, $ATR100_{CiC}/d$, and $ATR100_{tot}$ obtained by *AirClim* (true model value) with those obtained from the regression formulas (fit value). The color indicates flight distance. Grey lines indicate a perfect correlation.



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Since the regression formulas for the different clusters are independent from each other, mismatches at the cluster boundaries cannot be avoided. The solid lines in Figure 13 to Figure 15 indicate the climate effect at the cluster boundary calculated using the equations for either cluster for a flight with average NO_x emissions and fuel use. The difference between the solid lines indicates the mismatch. For average NO_x emissions and fuel use cases, the mismatch is never larger than a factor of two. Particularly large mismatches are found between the short-flight and the tropical cluster for flight with a mean latitude in the equatorial region, as well as for very long flight connections between the mid-latitude and tropical clusters. The figures also indicate the climate effect at the cluster boundary calculated using either cluster for flights with minimal and maximal NO_x emissions (dashed lines) and for flights with minimal and maximal fuel use (dotted lines).

In conclusion, the resulting regression formulas (Eq. 2-11) can be used in combination with their best-fit coefficients (Table 3) to efficiently compute the climate effect in terms of ATR100 of any flight with given distance, mean latitude, fuel use, and NO_x emissions without the need to run a climate response model.

Figure 13: ATR100 at the cluster boundary of 462 km computed from different clusters' regression formulas under five different sets of conditions: average NO_x emissions and fuel use, high and low NO_x emissions, as well as high and low fuel use. Average conditions are taken as the average from all flight connections in a region around the boundary, whereas high and low are obtained from the respective maximum and minimum values.

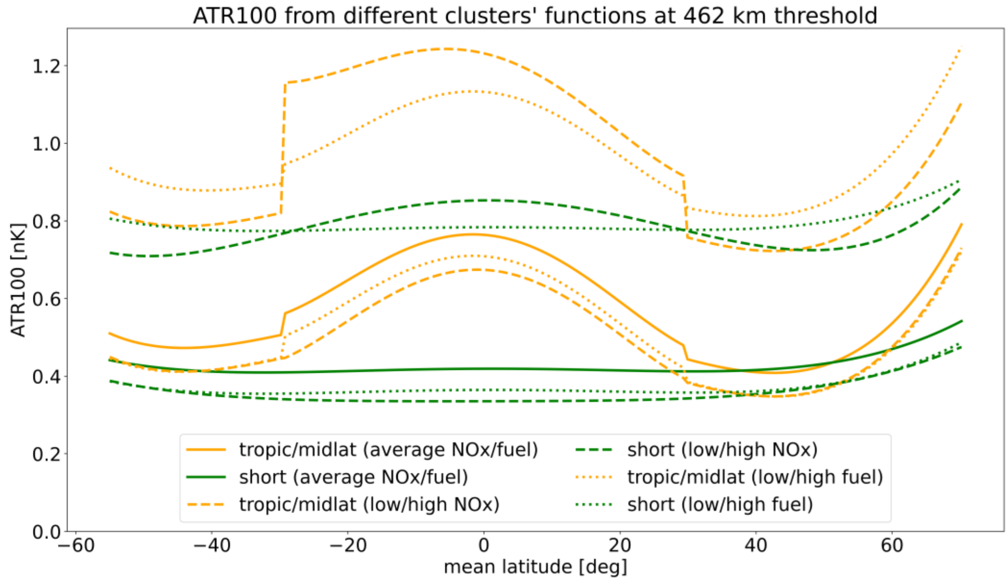

Figure 14: Same as Fig. 9, but for the cluster boundary at 29.7°N values.

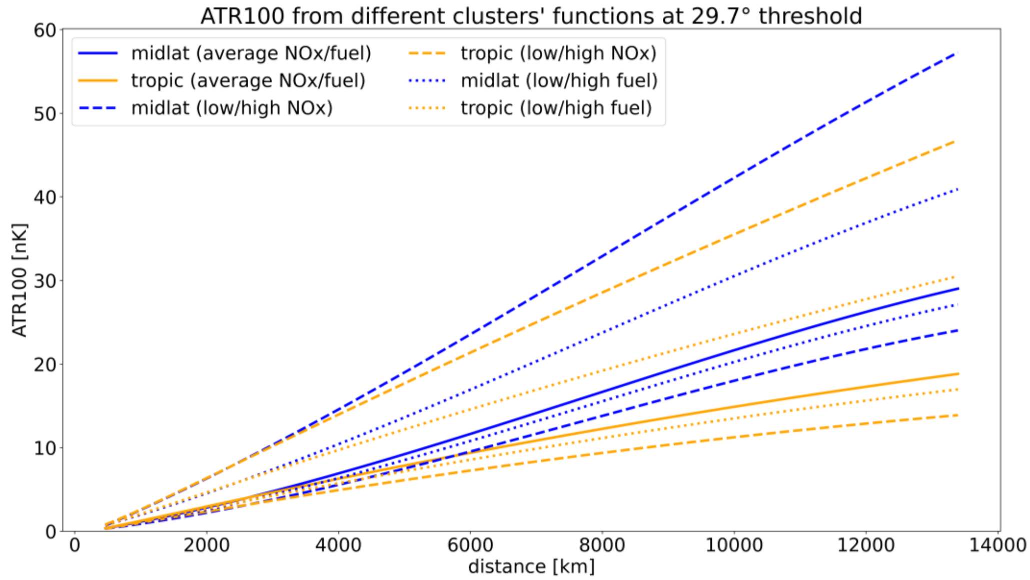

Figure 15: Same as Fig. 9, but for the cluster boundary at 29.7°S values.

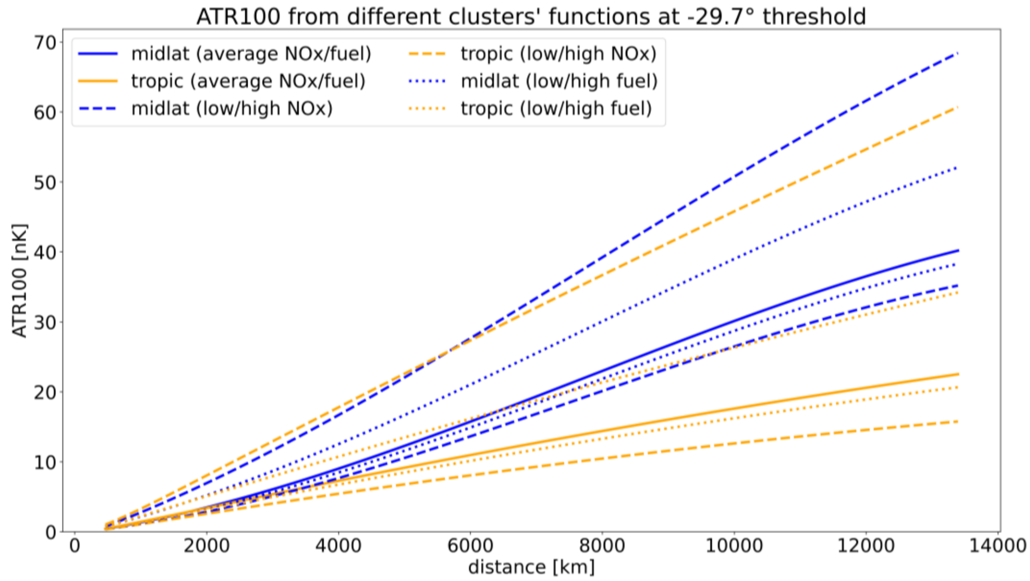

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Table 3: Best fit solutions for CO2e regression formulas. Coefficients for NO_x are in units of mK / kg(NO_2), coefficients for H_2O are in units of mK / kg(fuel), and coefficients for H_2O are in units of mK / km

Cluster quantity	short-flight			mid-latitude			tropical		
	NO_x	H_2O	CiC	NO_x	H_2O	CiC	NO_x	H_2O	CiC
0	2.00E-15	9.03E-13	4.56E-19	4.79E-04	1.12E-12	2.57E-21	1.41E-01	4.64E-13	3.59E-05
1	-7.14E-14	-	-1.96E-17	1.29E02	1.44E-03	-5.84E-17	1.16E-03	1.35E-03	2.19E01
2	2.37E-04	-	-1.46E-14	5.28E-14	5.91E-03	-3.03E-14	4.93E-02	1.72E-02	-1.91E-13
3	1.54E-04	-	-	-7.52E-04	4.86	-1.37E-03	6.06E-12	6.66	-5.64E-05
4	-1.46	-	-	-	-	-1.18E-02	-2.90E-10	-	5.92E-07
5	1.17	-	-	-	-	5.45	5.03E-08	-	-1.64E-03
6	6.47E03	-	-	-	-	5.03E01	-	-	1.14
7	-	-	-	-	-	-7.73E03	-	-	-

4 User guide

For simplifying the estimation of CO_2 equivalents per flight, resulting regression formulas for fuel, NO_x and CO2e were embedded into an Excel application. The basic user version of the Excel application consists of three Excel sheets: “Info” (see “A” in Figure 16), “Calculator” (“B”) and “AirportDatabase” (“C”):

a) The “Info” sheet provides general information such as the release date and the version number. In addition, you will find an instruction for the use of DLR's simplified CO_2 equivalent Estimator and an exclusion of liability.

b) The “Calculator” sheet is the core of the application. All input values are entered in this sheet (see Section 4.1) and all calculation results are displayed (see Section 4.2).

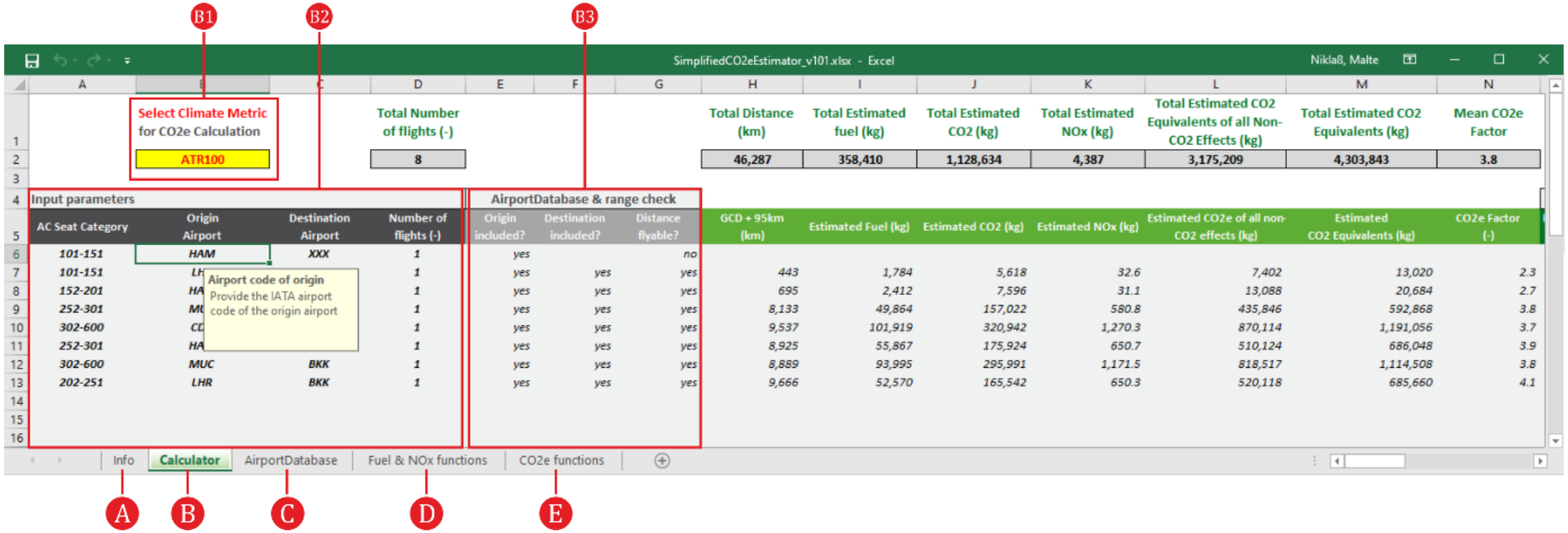
c) The “AirportDatabase” provides detailed position information for almost 9.000 airports. Airports are identified via the IATA airport code, which is a three-letter geocode defined by the International Air Transport Association (IATA). If the desired airports are not included in the "AirportDatabase" sheet, users are free to add them.

In the developer version of the Excel application there are two more Excel sheets: Fuel & NO_x functions (see “D” in Figure 16) and “CO2e functions” (“E”)

d) In the “Fuel & NO_x functions” sheet, regression formulas and polynomial coefficients are stored for various aircraft classes. These formulas and coefficients are used for the calculation of the fuel consumption and the cruise emission index of nitrogen oxides.

e) The “CO2e functions” sheet provides all necessary formulas and polynomial coefficients for the carbon dioxide equivalent calculation. Formulas and coefficients are stored separately for the “short-flight”, “mid-latitude” and “tropical” cluster and differ according to the climate agent (CO_2, H_2O, NO_x, CiC) (see Chapter 3). In addition, conversion factors are stored here, which allow to express the CO2e either in the climate metric ATR_{100} (average temperature response over 100 years) or in $AGWP_{100}$ (absolute global warming potential over 100 years).

Figure 16: Graphical User Interface



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4.1 Input parameters

The calculation of CO_2 equivalents is based on following input parameters, which users enter into the "Calculator" spreadsheet of the Excel application (see “B1” and “B2” in Figure 16):

1. Selection of the preferred climate metric for the calculation of CO_2 equivalents in cell "B2". The drop-down list allows the user to choose between ATR_{100} or $AGWP_{100}$.
2. Selection of the preferred aircraft seat category in column “A”. A drop-down list allows the user to choose between five different seat categories. The proposed seat categories range from 101-151 seats to 302-600 seats and represent following aircraft types:
   101-151 seater: like Airbus A319, A320, Boeing 737
   152-201 seater: like Airbus A320, A321, Boeing 737, 757
   202-251 seater: like Airbus A330, Boeing 767, 777
   252-301 seater: like Airbus A330, A340, Boeing 777
   302-600 seater: like Airbus A340, A380, Boeing 747, 777
3. Enter the IATA airport code of the origin and destination airports in columns “B” and “C”. Columns “E” and “F” indicate whether the airports are in included in the "AirportDatabase" sheet or not (see “B3” in Figure 16). If one of the desired airports is not included, users are free to add it in the "AirportDatabase" sheet (“C” in Figure 16). Also indicated in the "G" column of the "Calculator" sheet is whether the selected origin-destination pair is flyable with the selected aircraft seat category.
4. The number of flights performed on the city pair connection is entered into column “D”. The value "1" is the minimum input value here.

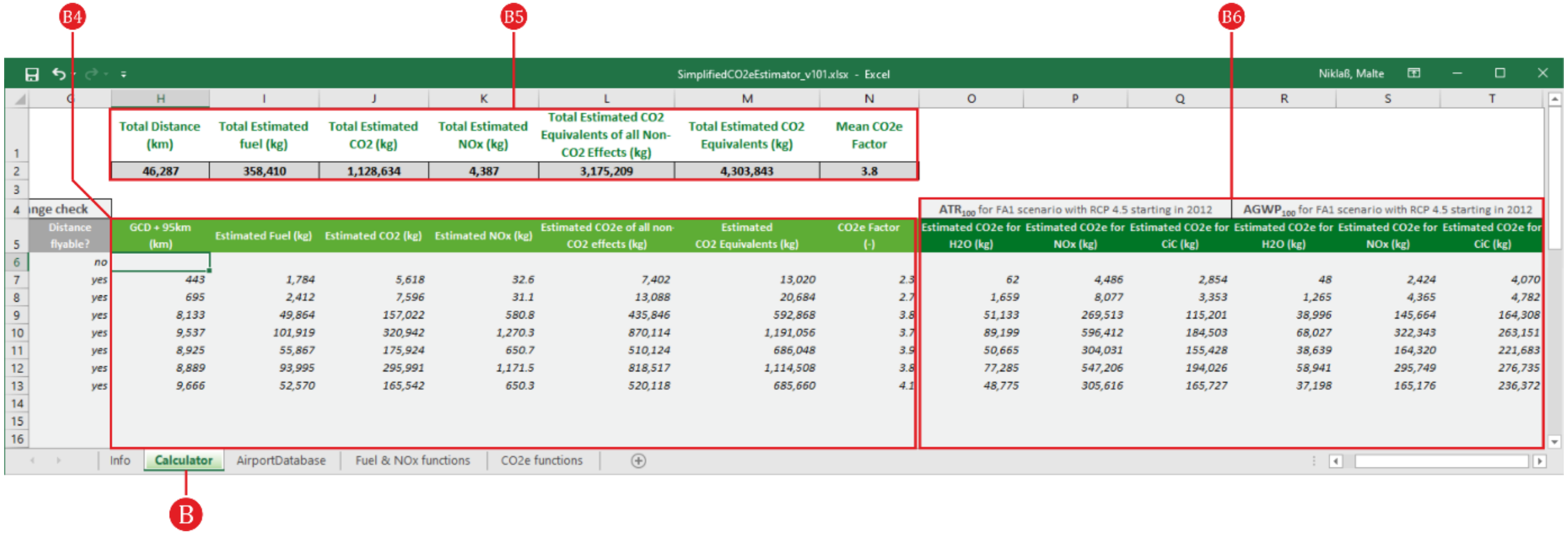
4.2 Output parameters

If all entries have been made correctly the “Simplified CO2e Estimator” will return the following output data in columns “H” to “T” of the “Calculator” sheet (see “B4” and “B6” in Figure 16):

- The great circle distance (GCD) plus 95km for arrival and departure procedures (in km),
- The fuel burn estimate (in kg),
- The estimated amount of CO_2 emissions (in kg),
- The estimated amount of NO_x emissions (in kg),
- The estimated CO_2 equivalents of H_2O, NO_x and CiC (in kg), expressed as ATR100 and AGWP100
- The estimated CO_2 equivalents of all non-CO_2 effects (in kg),
- The estimated CO_2 equivalents of all effects (CO_2 and non-CO_2 effects) (in kg),
- The estimated CO_2 equivalent factor of the flight (CO_2 equivalents / CO_2).

In row 2 the “Calculator” sheet, aggregated values for all flights are displayed for the distance, fuel consumption, emissions (CO_2, NO_x) and CO_2 equivalents (total value, value of all non-CO_2 effects, mean factor) (see “B5” in Figure 17).

Figure 17: Graphical User Interface part 2



5 Summary

Within this study, an application for a simplified estimate of CO_2 equivalents per flights has been developed. The simplified calculation method estimates non-CO_2 climate effects of air traffic as precisely as possible, without detail information of the actual flight route, actual fuel burn and the current weather situation. For this purpose, we evaluated a data set containing a global set of detailed flight trajectories, flight emissions and climate responses for various aircraft types. Based on the data set regression formulas for fuel consumption, NO_x emissions and climate responses have been generated.

In order to increase the accuracy of CO2e regressions formulas, flight connections were clustered using the K-Means clustering algorithm. The resulting three clusters have distinct characteristics. The short-flight cluster (green) has a negligible contribution of contrails to the climate effect, and a strong contribution of CO_2. Flight connections in this cluster often do not reach sufficient altitudes for contrail formation. The climate effect of the tropical cluster (orange) is dominated by contrails because contrails have a particularly large climate effect in the tropics. The mid-latitude cluster (blue) contains the remaining flight connections and has large climate effect contributions from NO_x and H_2O.

By deriving regression formulas for each of the simplified clusters, the mean absolute relative error of all flights and aircraft types was reduced to 15.0%, which represents the *AirClim* computations 5% better than the CO2e regression formulas of Dahlmann et al. (2021) for the A330-200 aircraft. The new mean absolute relative error is 9.4% for the short-flight cluster, 16.1% for the mid-latitude cluster, and 15.0% for the tropical cluster. Since the regression formulas for the different clusters are independent from each other, mismatches at the cluster boundaries cannot be avoided. For average NO_x emissions and fuel use cases, the mismatch is never larger than a factor of two. Particularly large mismatches are found between the short-flight and the tropical cluster for flight with a mean latitude in the equatorial region, as well as for very long flight connections between the mid-latitude and tropical clusters.

For simplifying the estimation of CO_2 equivalents per flight, resulting regression formulas for fuel, EINOx and CO2e were embedded into an Excel application called “Simplified CO2e estimator”. After selecting the preferred input values (climate metric, aircraft seat category, origin and destination airports, flight frequency), the tool returns

- the great circle distance (GCD) plus 95km for arrival and departure procedures (in km),
- a fuel burn estimate (in kg),
- estimated CO_2 and NO_x emissions (in kg), and
- CO_2 equivalents for H_2O, NO_x and CiC.

The level of the CO2e factor strongly dependents on the level of the CO_2 reference. Since the simplified estimate of CO_2 equivalents is designed for ecological footprint assessments of present and future flights, we do not consider any emissions of historic aviation. As the climate impact of CO_2 is more affected by the historical emission than short lived non-CO_2 effects, the relation between non-CO_2 effects and CO_2 is higher than the known factor from the literature for non-CO_2 effects of 2-3, which is based on the total CO_2 level from preindustrial times (e.g. from 1940 to 2018 for Lee et al., 2021).

This simplified estimate of CO_2 equivalents is not designed for use in an emissions trading system but could also be applied for plausibility checks or as a backup when airlines are unable to provide the required data.

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