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Uncertainty Quantification of Contrail Climate Impacts using Non-Intrusive Polynomial Chaos

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Objective

The work will answer: **How does uncertainty in the weather change the estimated impacts of contrails** on the climate in terms of total global radiative forcing (RF), and the benefits of using sustainable aviation fuels (SAF)?

Background

Persistent contrails act as contributors to total climate change.[1]

The climate impact of contrails can be represented as a radiative forcing (RF), which depends on contrail optical and physical properties, which are in turn impacted by meteorological conditions.[2]

Uncertainties in meteorological data affect our ability to predict contrail RF effects.[3] Quantifying the sources and effects of meteorological uncertainty on contrail RF improves our ability to predict and mitigate contrail impacts.

Current uncertainty analysis largely focuses on meteorological data sample error,[4] but these methods do not provide large sample sizes[5,6] of contrail properties at practical computational cost.

This work addresses this shortcoming by introducing a non-intrusive method for sampling the contrail property space efficiently under differing conditions (Polynomial Chaos Expansion, PCE).

Acknowledgements
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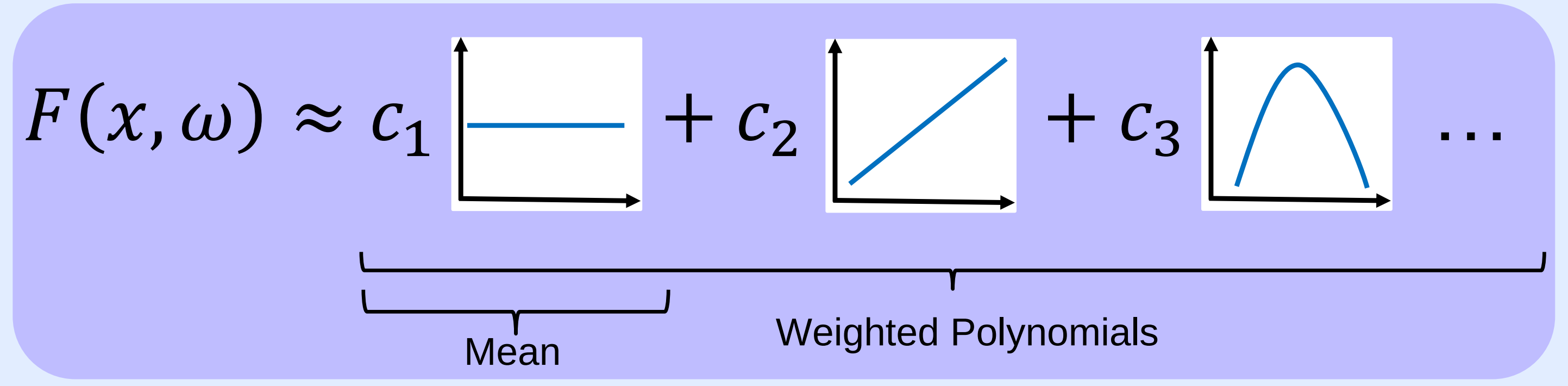
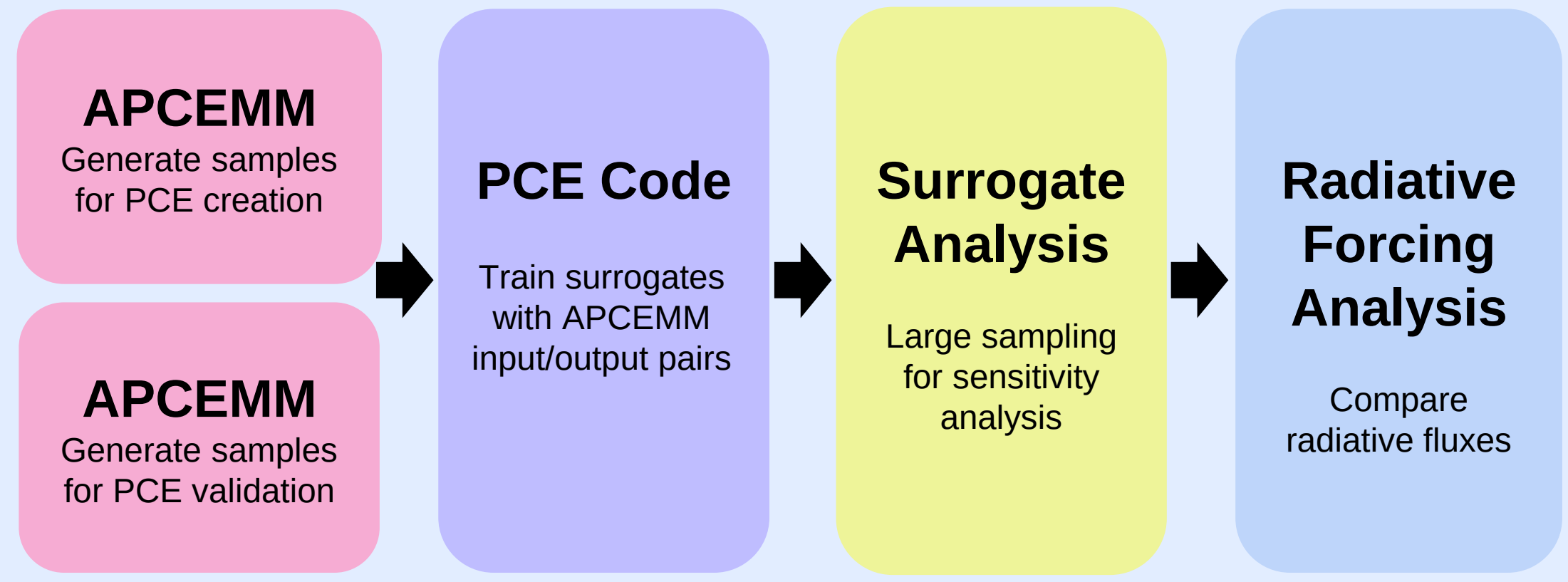
Methods

Polynomial Chaos Expansion (PCE) and Overview

The scenario space requires large sample sizes to perform uncertainty propagation and sensitivity analysis of a variable and uncertain system. Each variability introduced requires new analysis accounting for said variability. A surrogate model approximates a computationally expensive model and allows for accurate and fast evaluation of the expensive model. PCE is a technique to construct surrogate models (F) by summing combinations of polynomials [Fig. 1]. The basis for our surrogates is the computationally expensive Aircraft Plume Chemistry Emission and Microphysics Model (APCEMM). An overview of the workflow is shown on the right.





APCEMM
Generate samples for PCE creation

APCEMM
Generate samples for PCE validation

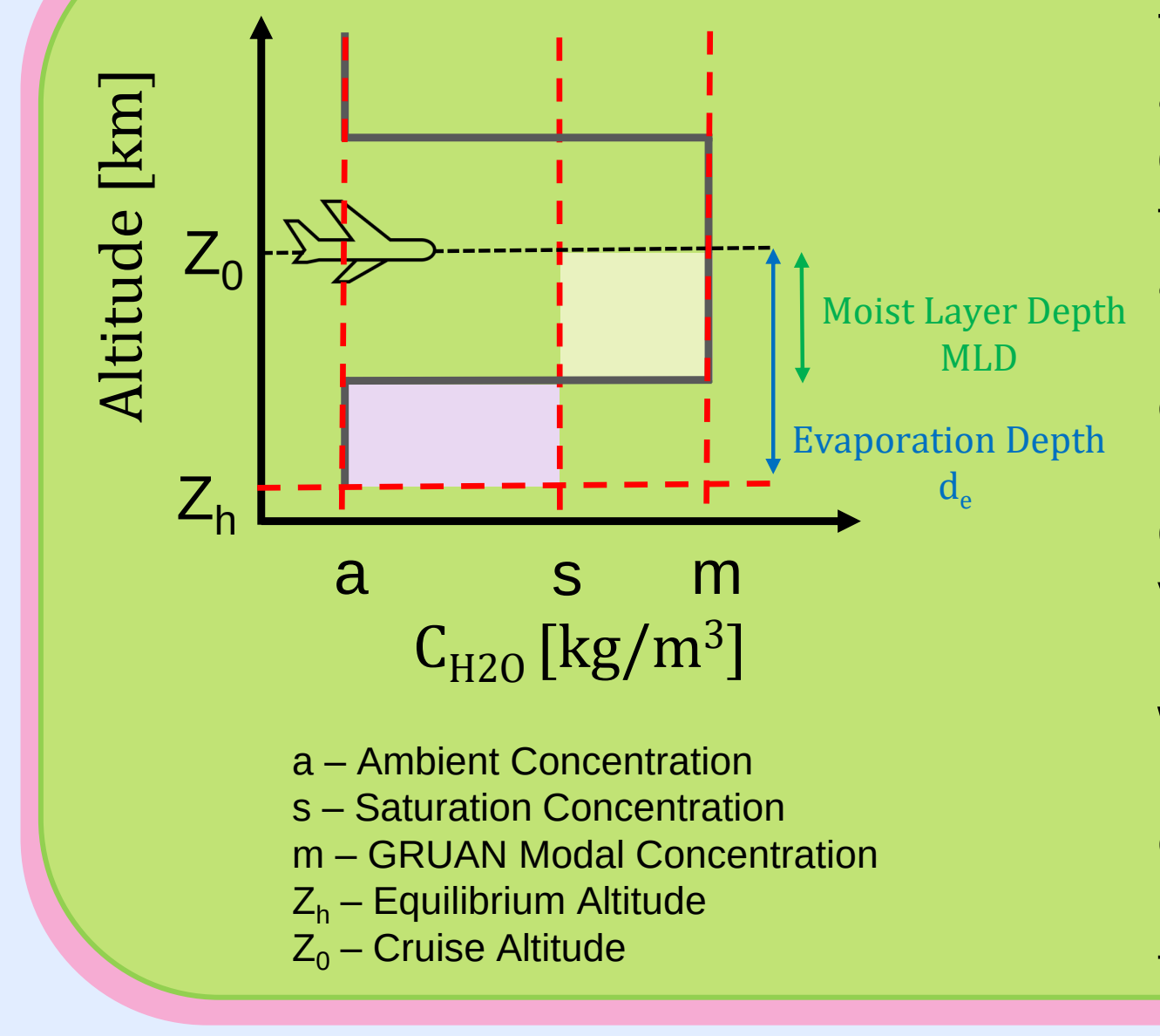
PCE Code
Train surrogates with APCEMM input/output pairs

Surrogate Analysis
Large sampling for sensitivity analysis

Radiative Forcing Analysis
Compare radiative fluxes

1) Contrail Property Estimation and Modelling

Even assuming data is perfectly collected there is post-processing uncertainty, like grid-size. Data is not collected and processed with 100% accuracy: Meteorological datasets have wet and dry biases that incur additional uncertainty[4]. These uncertainties are represented by the APCEMM properties moist-layer depth (MLD), supersaturated relative humidity (RH_{sps}), and time-to-mixing (TTM). Fuel blend also influences contrail radiative forcing effects. Soot particle number, soot size distribution, and sulfur content contribute to ice nucleation and growth, i.e. contrail formation and persistence.



a – Ambient Concentration
s – Saturation Concentration
m – GRUAN Modal Concentration
Z_h – Equilibrium Altitude
Z_0 – Cruise Altitude

Figure 1: **MLD and other key parameters**
The uncertainties introduced by meteorological data are represented as APCEMM input properties. The depth of supersaturation is the MLD, captured using the global modes of radiosonde measurements of atmospheric conditions, GRUAN. Ambient RH and RH_{sps}, combined with the MLD, define external conditions for the contrail. The means of the respective probability density functions (PDFs) are determined with GRUAN modal data, while the variance is computed by the spread of data over both GRUAN and ERA5 data. This incorporates the wet and dry bias of both meteorological datasets into the PDFs. TTM represents the time before the contrail region begins mixing with subsaturated air by way of shear, diffusion, and temperature fluctuations.

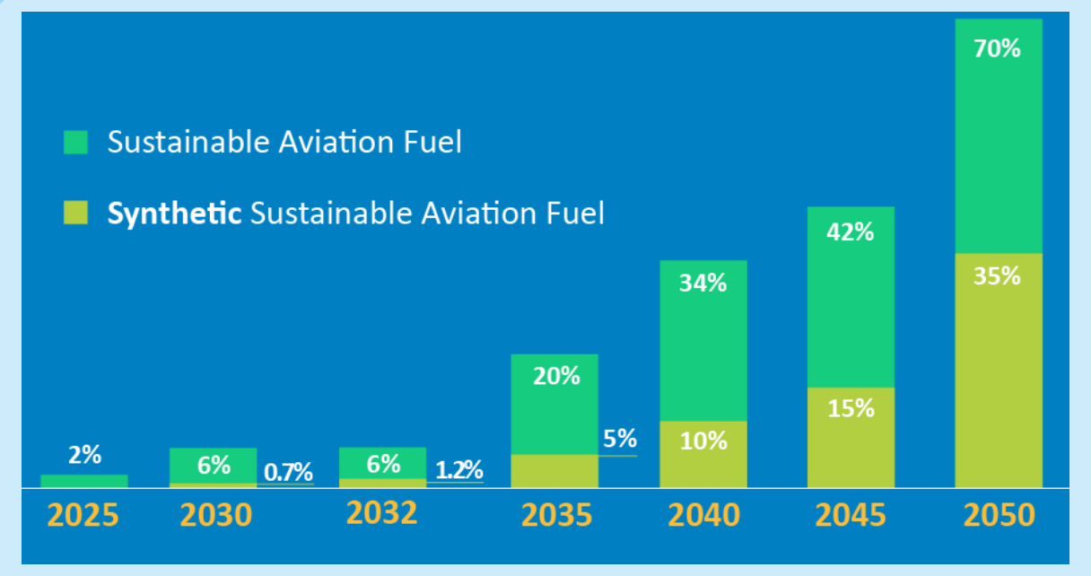


Figure 3: **ReFuelEU SAF milestones**
Analyzing proposed ReFuelEU SAF blends provides insight on future contrail impact sensitivity.

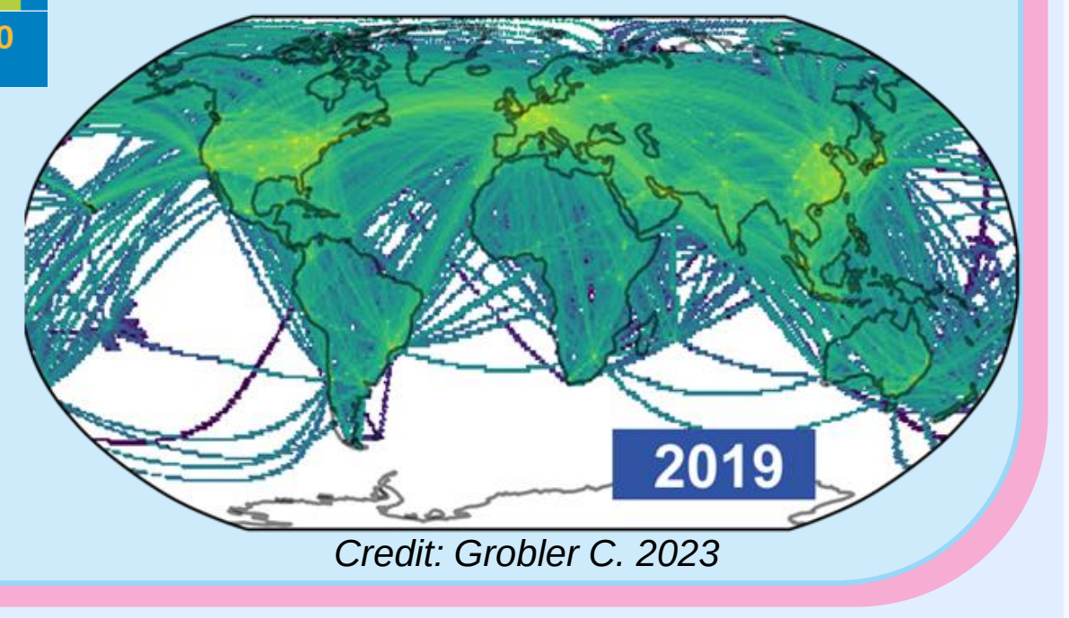


Figure 2: **2019 flight paths, colorized by fuel burn**
Top 5 flight-aircraft pairs chosen by cruise kilometers flown in 2019.

Credit: Grobler C. 2023

2) PCE and Surrogate Application

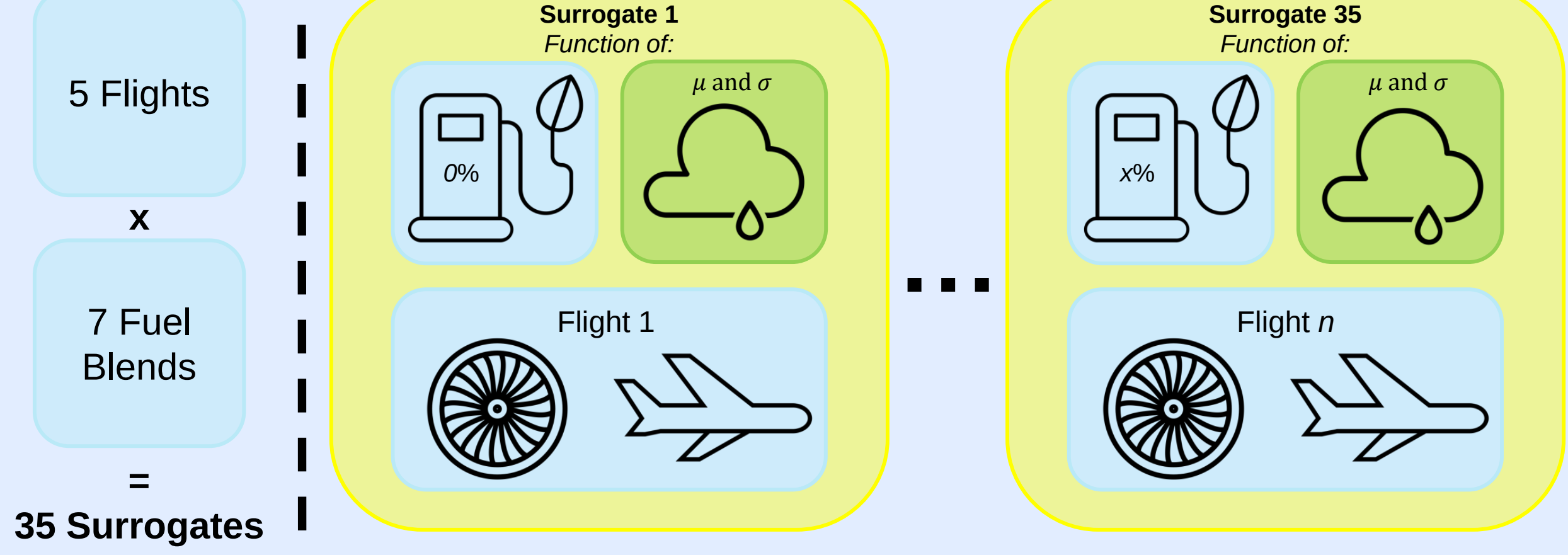


Figure 4: **Variable and uncertain parameters informing PCE surrogate**
The fuel blend percentage and engine/aircraft pair individualize each surrogate (variable, not uncertain). The meteorological properties are uncertain, but uniform across the surrogates (uncertain, not variable). Fast evaluation of the surrogate allows for Saltelli sensitivity analysis: Using a “pick and freeze” estimator, if a random variable X_i is (not) influential then the computed value of S_i will be (small) large. This computation requires $M(p+2)$ evaluations in comparison to pM^2 for a Monte Carlo approach. *(M: Independent realizations of inputs, p: Number of uncertain parameters)*

3) Radiative Forcing Calculation

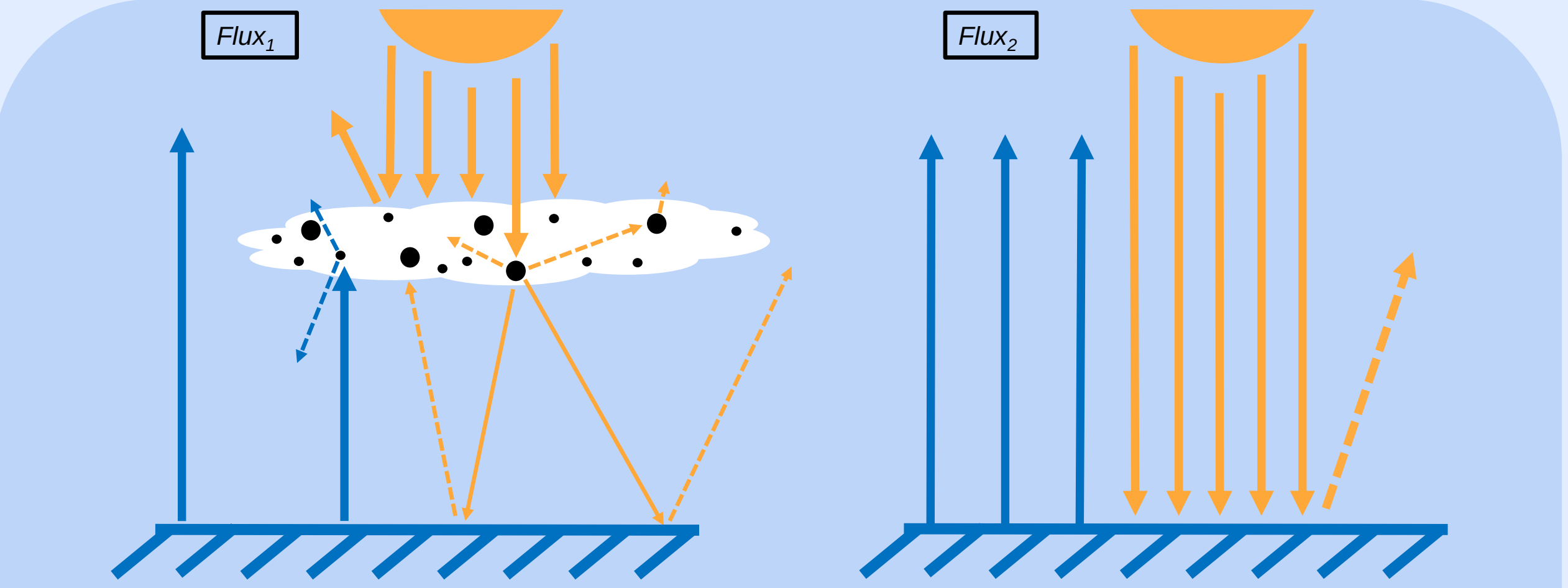


Figure 5: **Radiative flux dependence on contrail properties**
LibRadTran calculates Mie scattering, absorption, and emission properties of the simulated contrails, resulting in an RF estimation. RF is computed where $Flux_1$ is calculated clear-sky with a contrail present at 12pm over ocean conditions (Left) and $Flux_2$ is calculated clear-sky with no contrail present over ocean conditions (Right). Both scenarios use the meteorological conditions associated with the surrogate. Calculating the RF effect cumulatively for all flights operating with the aircraft-engine combinations studied for the year 2019 produces a PDF of global RF effects as a function of SAF blend, MLD, RH_{sps}, and TTM.

Preliminary Results

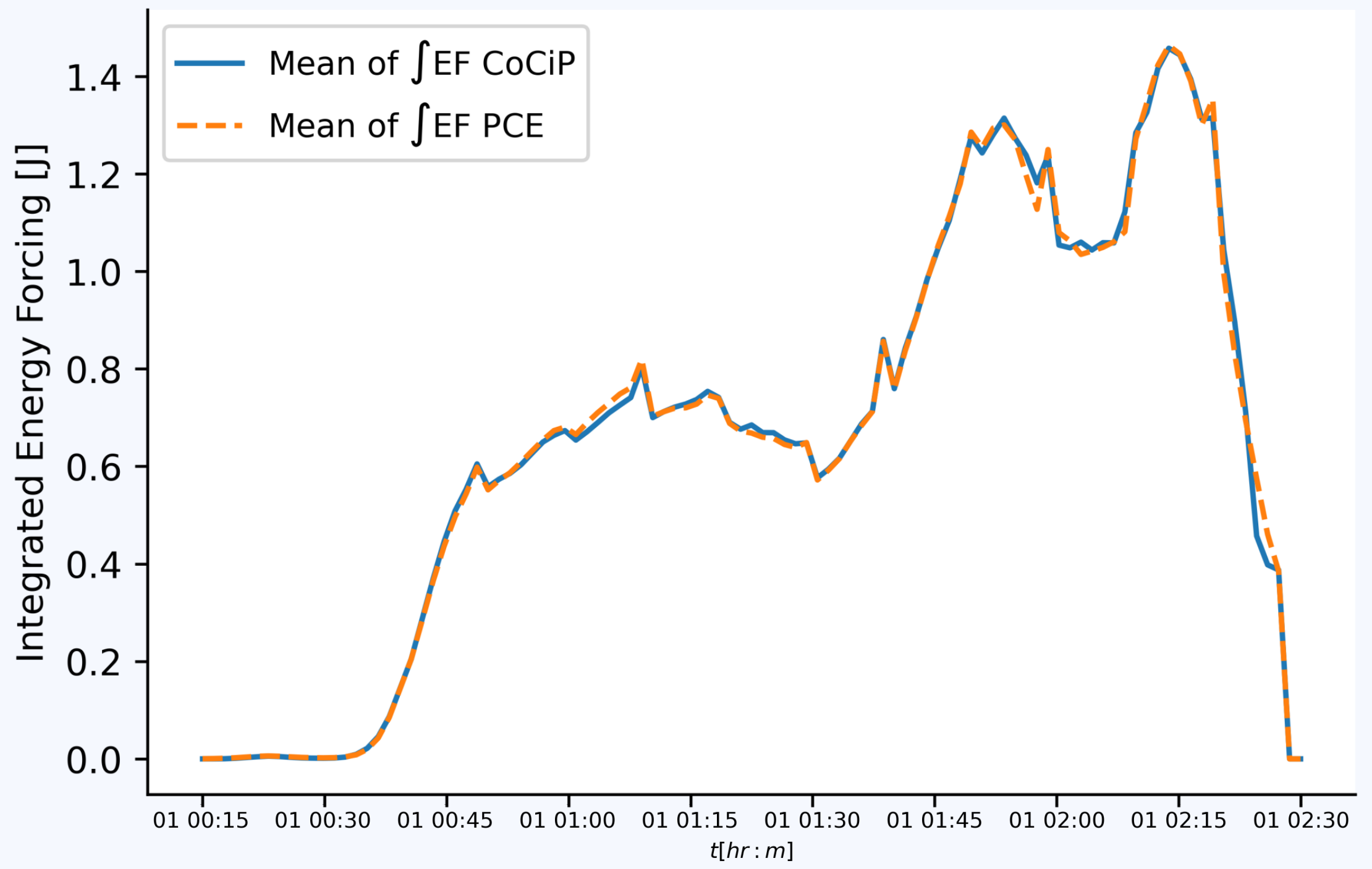


Figure 6: **Preliminary estimates of contrail properties (energy forcing, EF) using PCE with the Contrail Cirrus Prediction Model (CoCiP)**
To showcase the PCE and surrogate method, a test case using the less computationally expensive contrail modelling program CoCiP was built. The L^2 error associated with this test case is 3.94. This acts as a proof of concept for the PCE and surrogate methods selected.

Next Steps

- Complete surrogate training datasets (APCEMM runs)
- Describe MLD and RH_{sps} uncertainty coupling
- Determine TTM key dependencies
- Compare mean and variance when using different fuels and different aircraft
- Calculate sample-set estimate of TTM mean and variance
- Integrate conversion from APCEMM outputted integrated OD to LibRadTran radiative forcing
- Perform Saltelli sensitivity analysis and L^2 error analysis on APCEMM surrogate results

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