<u>Uncertainty-Aware and Explainable Sequential Planning for Operational Contrail Mitigation</u>

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Background: Aviation's non-CO_2 climate impacts remain a major scientific, environmental, and operational challenge. Persistent contrails and contrail cirrus, which form when aircraft exhaust encounters ice-supersaturated air, contribute a disproportionately large share of aviation's near-term radiative forcing. Global analyses show that ~2% of flights account for ~80% of contrail energy forcing [1], indicating strong potential for targeted mitigation. Field trials such as the Google–American Airlines demonstration have shown that modest altitude adjustments can reduce contrail formation by >50% with only 1–2% fuel penalties [2]. While higher-efficiency engines require long-term technology development, near-term contrail-aware operational adjustments offer immediate climate benefits.

However, the physical and statistical characterization of contrail formation remains deeply uncertain. Numerical Weather Prediction (NWP) models rely on humidity observations with limited spatial and vertical fidelity [3]. Ice-supersaturated regions (ISSRs) are especially difficult to predict: radiosonde measurements, satellite retrievals, and reanalysis products often disagree, and ensemble forecasts frequently miss fine-scale humidity structure [3, 4, 10]. Systematic moist biases persist across observing systems, and upper-tropospheric humidity remains one of the least well-constrained meteorological variables [10]. Satellite detection and attribution introduce additional uncertainty due to spatial resolution, viewing geometry, cloud overlap, and the inherently 2-D nature of imagery [4]. These limitations affect assessment of layer depth, ISSR structure, microphysical evolution, and ultimately radiative forcing. Most existing operational assessments rely on deterministic thresholds that cannot represent these uncertainties or model-form errors in tools such as CoCiP. Prior work has advanced detection, microphysical modeling, and operational demonstrations [1, 4], but these components have evolved independently.

Meanwhile, the policy and regulatory environment is shifting rapidly. The EU plans non-CO_2 monitoring requirements by 2027 [5], European ANSPs are exploring contrail-aware trajectory planning [6], and ICAO and the FAA Contrails Research Roadmap (2025) emphasize the need for methods that explicitly incorporate atmospheric uncertainty, model discrepancy, observational limitations, and operational feasibility [7]. Because transatlantic routes dominate contrail-susceptible operations, there is a need for a research-grade uncertainty quantification (UQ) and Bayesian decision framework that integrates heterogeneous atmospheric data, physical models, and sequential operational evaluation.

Proposal: My objective is to develop an uncertainty-aware and explainable Bayesian inference and decision layer that integrates atmospheric detection, physical modeling, heterogeneous data assimilation, and sequential operational mitigation. Informed by advances in contrail physics, UQ, atmospheric science, and experiment design [1, 4, 12], I aim to create a unified planning framework that: (1) builds a calibrated probabilistic surrogate of contrail physics that accounts for model-form discrepancy and heterogeneous atmospheric and satellite data, (2) embeds this surrogate within a Bayesian sequential decision framework under partial observability, and (3) evaluates performance using a statistically principled paired-difference experimental design.

Beyond the application of contrail mitigation, the broader goal is to contribute to methodology in uncertainty quantification and Bayesian computation for complex environmental and operational systems, especially in Bayesian surrogate modeling under model discrepancy, uncertainty decomposition and data assimilation for multi-source atmospheric datasets, and risk-sensitive sequential decision-making under epistemic and aleatory uncertainty.

Aim 1: Develop a calibrated probabilistic surrogate of CoCiP incorporating atmospheric and fuel-dependent uncertainty: I will develop a probabilistic surrogate of the CoCiP contrail–cirrus model that explicitly models multiple sources of uncertainty: input uncertainty (humidity, temperature, winds), parametric uncertainty (microphysical and emissions-related parameters), and model-form discrepancy between CoCiP and reality.

Using CoCiP/pycontrails [8], I will simulate contrail formation and radiative forcing across representative meteorological regimes, pairing each segment with NWP ensemble forecasts, reanalysis datasets, and satellite-informed humidity products (e.g., GOES-R cloud-top retrievals, AIRS/IASI humidity profiles). This supports stronger characterization of upper-tropospheric humidity, ISSR layer depth, and supersaturation persistence. Calibration will be formulated as a Bayesian inverse problem where uncertain parameters (e.g., humidity bias corrections, ice-nucleation efficiencies, emissions-scaling factors) are inferred from atmospheric and satellite datasets [4, 9–11].

Because high-fidelity exhaust composition data are limited, I will vary only fuel properties (SAF blends, aromatic/sulfur content) while fixing engine-cycle parameters. Engine-cycle and fuel-dependent exhaust variables (nvPM indices, exhaust-temperature and velocity proxies, water vapor, aromatic/sulfur content) will be incorporated at literature-supported fidelity. Model-form discrepancy will be represented using a low-dimensional structured Gaussian-process prior to ensure identifiability. A Bayesian ensemble or Bayesian neural network surrogate will jointly emulate CoCiP outputs (e.g., contrail-formation probability, persistence, radiative-forcing proxies) and discrepancy terms. Performance will be assessed via probabilistic calibration metrics (Brier score, CRPS) and uncertainty decomposition across atmospheric, parametric, and discrepancy sources.

This aim focuses on developing methodological components for Bayesian surrogate modeling under model discrepancy, multi-source atmospheric data assimilation, and structured uncertainty decomposition in contrail-relevant predictions.

Aim 2: Formulate an uncertainty-aware, explainable Bayesian sequential planner: Contrail mitigation is fundamentally a Bayesian decision problem under partial observability, heterogeneous data, and model-form misspecification. Rather than assessing isolated points along a route, the proposed framework performs sequential optimization over feasible trajectory adjustments using look-ahead to balance atmospheric risk with operational feasibility. I will formulate the task as a partially observed Markov decision process (POMDP) and develop a hybrid planner combining a policy-learning component proposing feasible operational maneuvers, Monte Carlo Tree Search (MCTS) for downstream evaluation under ensemble meteorology and surrogate uncertainty, and risk-sensitive objectives (CVaR) to guard against overconfident decisions in high-uncertainty regions.

Meteorological variability will be incorporated using ensemble forecasts and reanalysis spread to represent structured atmospheric scenarios, not calibrated probability distributions. Surrogate-model and model-form uncertainty enter through Aim 1. Operational uncertainty (navigation deviations, dispatch-related offsets) will be represented as bounded stochastic perturbations in the transition model.

All three uncertainty types will be propagated through MCTS rollouts. Explainability will be achieved using variance decomposition and attribution tools (SHAP, integrated gradients), enabling the planner to distinguish whether high predicted contrail risk arises from atmospheric variability, surrogate uncertainty, model discrepancy, or uninformative humidity forecasts. Counterfactual analyses will clarify how small changes in atmospheric assumptions or fuel properties alter recommended actions. This aim focuses on methods for Bayesian decision-making under model discrepancy, sequential planning in partially observed environmental systems, and interpretable decision-support in climate-relevant contexts.

Aim 3: Evaluate the framework using paired-difference experimental design and multi-dataset atmospheric comparisons: Evaluation will use the paired-difference methodology developed in recent MIT LAE contrail-avoidance studies [12], providing a controlled-trial structure for estimating treatment effects. Retrospective analyses will compare baseline and planner-modified trajectories using CoCiP (with the calibrated surrogate and discrepancy model) for radiative forcing estimation and satellite detections where available. Metrics include deviation length, contrail-impact reduction, humidity-regime sensitivity, and system-level treatment effects (ESTE/EATE). Validation will emphasize radiative-forcing proxies and humidity diagnostics by comparing surrogate outputs against ERA5, AIRS/IASI, and other satellite humidity datasets. Synoptic-scale drivers of ISSRs (UTLS humidity variability, tropopause structure, jet-stream dynamics) will be analyzed to contextualize performance across meteorological regimes.

This aim focuses on connecting Bayesian experimental design, causal treatment-effect estimation, and environmental uncertainty quantification in a complex, data-limited physical system.

Integration/Expected Contributions: Together, these aims create a unified Bayesian inference and decision framework that links atmospheric uncertainty, surrogate physical modeling, and sequential evaluation. By propagating meteorological, parametric, and model-form uncertainty, and distinguishing them from operational variability, the system will identify when mitigation strategies are supported by the available evidence and when uncertainty dominates predicted outcomes. The surrogate's ability to incorporate fuel-dependent emissions parameters, heterogeneous atmospheric datasets, and structured model discrepancy allows the framework to adapt as new observations and microphysical insights emerge. More broadly, the integration of Bayesian surrogate modeling, inverse problems, data assimilation, and sequential decision-making offers a generalizable methodology for analyzing trajectory-dependent environmental processes in high-dimensional, uncertain state spaces.

Aviation is a highly relevant representative system in which physical processes, observational limitations, operational constraints, and policy considerations interact in ways that challenge conventional modeling and decision-making. The methods developed here, probabilistic surrogates that account for model-form discrepancy, multi-source data assimilation under structurally biased observations, and sequential planning in partially observed and dynamically uncertain environments, are broadly relevant to environmental and infrastructure systems where decisions must be made with imperfect information. Similar challenges arise in renewable-energy integration, grid operations, air-quality forecasting, and other climate-relevant applications in which uncertainty is high, data sources conflict, and physical and operational models must be reconciled. By focusing on interpretable, uncertainty-aware evaluation and decision-support, this work aims to provide a set of tools that remain robust when observational fidelity is limited, physical models are imperfect, and operational feasibility is a binding constraint.

Challenges and Limitations:

<u>Humidity and ISSR uncertainty:</u> Upper-tropospheric humidity is poorly constrained; the framework is built to function under these limits and incorporate higher-fidelity data as they emerge.

Observational limitations: Satellite humidity products contain structural biases and geometric ambiguities; the framework will quantify disagreement across datasets.

<u>Model-form uncertainty:</u> CoCiP microphysical and radiative uncertainties will be handled through focused calibration and a structured discrepancy model.

<u>Computational cost:</u> Bayesian ensembles and MCTS are expensive; feasibility comes from reduced-order ensembles, limited maneuver sets, and explicit compute budgets.

References:

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