Table 2.1. DISCOVER-AQ Science Traceability Matrix

Science Objectives, Associated Questions, and Expected Outcomes	Scientific Measurement Requirements	Instrument Functional Requirements*	Investigation Functional Requirements	Modeling and Analysis Tools
Objective 1: Relate column observations to surface conditions for aerosols and key trace gases O_3, NO_2, and CH_2O ***A:*** *How well do column and surface observations correlate?* ***B:*** *What additional variables (e.g., boundary layer depth, humidity, surface type) appear to influence these correlations?* ***C:*** *On what spatial scale is information about these variables needed (e.g., 5 km, 10 km, 100 km) to interpret column measurements?* **Outcome:** Improved understanding of the extent to which column observations (as observed from space) can be used to diagnose surface conditions	Concurrent, urban-scale observations of column and in situ aerosols, O_3, NO_2, and CH_2O from aircraft and ground sites Observations of boundary layer depth, T, winds, and water vapor (column and profiles)	Active remote sensing of aerosols between surface and aircraft level with horizontal and vertical resolution of 1 km and 60m (backscatter and depolarization) Passive remote sensing of trace gas columns between surface and aircraft level to determine column amounts with spatial resolution of a few kilometers or better Airborne in situ observation of aerosol and trace gas profiles through the boundary layer and into the lower free troposphere at 1 hz (~5 m vert. and ~100 m hor. res. at nominal flight speeds) Passive remote sensing of total columns for trace gases and aerosol optical depth and in situ measurements of key trace gases and aerosols from a regional surface network with 10 minute resolution Ground-based, vertically-pointing lidar observations with 10 m and 10 minute resolution to provide 24-hour monitoring of aerosol profiles *Specific instrument capabilities are listed in Tables 3.1-3.7	Level flight in the mid-to-upper troposphere with a dedicated aircraft observing trace gas columns (passive) and aerosol distribution/BL depth (active) beneath the aircraft Airborne profiling with a dedicated platform to observe in situ vertical distribution of key trace gases, humidity, and boundary layer depth Distributed surface network to provide in situ and total column observations for key trace gases and aerosols One or more ground-based lidars to provide aerosol profiles	Multivariate statistical analysis to assess overall correlation between column and surface observations as well as sensitivity to location, time of day, boundary layer depth and mixing, humidity, surface and cloud optical properties, etc. Retrieval models capable of reanalysis of remote sensing measurements including information at a range of spatial resolution
Objective 2: Characterize differences in diurnal variation of surface and column observations for key trace gases and aerosols ***A:*** *How do column and surface observations differ in their diurnal variation?* ***B:*** *How do emissions, boundary layer mixing, synoptic transport, and chemistry interact to affect these differences?* ***C:*** *Do column and surface conditions tend to correlate better for certain times of day?* **Outcome:** Improved understanding of diurnal variability as it influences the interpretation of satellite observations from both LEO and GEO perspectives and improved knowledge of the factors controlling diurnal variability for testing and improving models	Continuous observation of column and in situ aerosols, O_3, NO_2, and CH_2O throughout daylight hours Key trace gas and aerosol observations identifying the influence of source emissions and chemistry (e.g., CO, CO_2, CH_4, reactive nitrogen, aerosol inorganic and organic composition)		All of the above plus: 8 hours of flight per day by both aircraft to observe column and profile evolution throughout daylight hours to include morning/evening rush hour emissions Observation of trace gas total columns at surface locations throughout daylight hours 24-hour observation of in situ trace gases and lidar aerosol profiles	All of the above plus: Regional chemical transport modeling to assess model capability to represent key meteorological parameters affecting column-surface correlations and interpret the role of various emissions sources (e.g., transportation, industry, power generation) and meteorological processes in affecting column and surface variability throughout the day
Objective 3: Examine horizontal scales of variability affecting satellites and model calculations ***A:*** *How do different meteorological and chemical conditions cause variation in the spatial scales for urban plumes?* ***B:*** *What are typical gradients in key variables at scales finer than current satellite and model resolutions?* ***C:*** *How do these fine-scale gradients influence model calculations and assimilation of satellite observations?* **Outcome:** Improved interpretation of satellite observations in regions of steep gradients, improved representation of urban plumes in models, and more effective assimilation of satellite data by models	Observe horizontal gradients in column and in situ aerosols, O_3, NO_2, and CH_2O as well as pollution tracers CO, CO_2, CH_4, and reactive nitrogen		High spatial resolution observations collected along flight transects to resolve variability down to scales of 100 m. Extensive sampling for different locations to characterize variability due to changes in emission (e.g., day-of-week), meteorological parameters, surface optical parameters, and local topography	Statistical analysis of spatial variability to characterize expected sub-grid gradients for coarser resolution satellites and models Multi-scale modeling to assess influences of model resolution on nonlinear chemical processes