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A 0D aircraft engine emission model with detailed chemistry and soot microphysics

Chowdhury G. Moniruzzaman *, Fangqun Yu

Atmospheric Science Research Center, State University of New York at Albany, 251 Fuller Road, Albany, NY 12203, USA

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ABSTRACT

Aviation emission of gas phase pollutants and particulate matter contribute to global radiative forcing and regional air quality degradation near airports. It is important to understand the formation and time evolution of these pollutants inside aircraft engines to design strategies for emission reduction. A physics and chemistry based zero-dimensional (0D) gas parcel model with detailed jet fuel chemistry and soot microphysics has been developed to predict the time evolution, formation history, and emission index (EI) of key combustion gases and size-resolved soot particles of an aircraft engine. The model was applied to a CFM56-2-C1 aircraft engine for idle operating condition, for which comprehensive measured data from the Aircraft Particle Emissions eXperiment (APEX) campaign are available. The measured EI data of four major pollutants, including CO, NOx ($NO + NO_2$), total hydrocarbon (HC) mass, and soot mass, were used to optimize the model parameters. The model predicts the time evolution of concentration of CO, NOx, HC, soot size distribution, CO_2, H_2O, SO_2, NO, NO_2, HONO, HNO_3, SO_3, H_2SO_4, O_2, H, H_2, O, OH, HO_2, H_2O_2, and some HC species in the combustor and turbine. Reasonable agreement was found between the simulations and the measurements. It was found for idle operating condition that, for most of the combustion products, concentrations did not change significantly in the turbine and nozzle, however, HONO, H_2SO_4, and HO_2 concentrations did change by more than a factor of 10, while NOx, NO, NO_2, O, OH, soot particle mass and soot particle number by less than a factor of 2. The developed model is computationally efficient and can be used to, study detailed chemical and microphysical processes during combustion, investigate the effects of different fuel compositions and operating conditions on aircraft emissions, and assist air quality study near aircraft emission sources.

1. Introduction

The impact of aviation combustion emissions on global climate in the troposphere and lower stratosphere [1–3] and air quality near airports [4,5] is of great concern to the scientific community and policymakers. While aviation-emitted carbon dioxide (CO_2) contributes only ~1.6% to total anthropogenic radiative forcing (RF) [3], non-CO_2 aviation emission of gas phase compounds such as carbon monoxide (CO), nitrogen compounds, water vapor, sulfur compounds, polyaromatic hydrocarbons (PAHs), un-burnt organic hydrocarbons (HCs) and particulate matter (PM), such as soot and volatile particles, contribute to both climate effects, being responsible for ~4.9% of total anthropogenic RF [3], and regional air quality degradation. The detail emission data of these key chemical compounds and soot from aircraft engine are required to study the effects of aviation emissions on climate and regional air quality. Moreover, understanding the formation mechanisms of these key chemical compounds and soot in the combustor and post combustor region (turbine and nozzle) of an aircraft engine is necessary in order to design a combustor with reduced emissions. Emission prediction through combustion modeling is an important approach to advance such an understanding.

The ideal combustion model will be a three dimensional (3D) computational fluid dynamics (CFD) flow model which determines the temperature, fluid velocity, pressure, and concentration of gas and soot in 3D spatial coordinates. But 3D CFD modeling needs excessive computation time even for the highly simplified combustion chemistry of one reaction step and a small number (2)–(5) of chemical compounds. Hence, to study details chemistry and soot microphysics, the number of fluid flow dimensions (0D/1D, 2D, 3D), chemical reactions, and soot size bins need to be optimized to get reasonable results within a practical computation time period. The present model focuses on the inclusion of detailed chemistry and size-resolved soot microphysics in an aircraft engine combustor and, therefore, a 0D combustion model has been chosen.

Modeling the aircraft engine combustor is difficult because of the inhomogeneous air mass and various processes inside the combustor. The combustion products are transported towards three spatial dimensions by advection and diffusion which result in a 3D distribution of temperature and equivalence ratio (which is the ratio of the fuel–air mass ratio over the fuel–air stoichiometric

* Corresponding author. Fax: +1 518 437 8758.
E-mail address: monir@asrc.albany.edu (C.G. Moniruzzaman).

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Nomenclature

Abbreviations

0D	0 dimensional
1D	1 dimensional
2D	2 dimensional
3D	3 dimensional
APEX	Aircraft Particle Emissions eXperiment (campaign)
CFD	computational fluid dynamics
DCA	dilution and cooling air
DZ	dilution zone (of the combustor)
EI	emission index (g/kg-fuel)
ER	equivalence ratio
FSC	fuel sulfur content
HC	hydrocarbon
HACA	hydrogen-abstraction/carbon-addition
ICAO	International Civil Aviation Organization
MF	mass fraction
PAH	polyaromatic hydrocarbon
PFR	plug-flow reactor
PSR	perfectly-stirred reactor
RF	radiative forcing
PM	particulate material
PZ	primary zone (of the combustor)
PZ1	primary zone 1 (of the combustor)
PZ2	primary zone 2 (of the combustor)
PZDA	primary zone dilution air
PZH	primary zone hole (of the combustor)
TN	turbine and nozzle of the engine
SVPM	secondary volatile particle matter

Symbols

$c_{p,j}$	heat capacity of jth gas parcel (Joule/mol-K)
f	the ratio of the cumulative mass of the jth unmixed gas parcel at any time to the cumulative mass of the jth unmixed gas parcel at the PZ1 end
$f_{da,pzh}$	the ratio of PZH air mass added as dilution air into the PZH section through PZH to the cumulative air mass at the end of the PZ2
FA_{ce}	the cumulative fuel air mass ratio at the end of the combustor (or the ratio of cumulative fuel flow rate to cumulative air flow rate at the combustor end)
$f_{j,ce}$	the ratio of the cumulative mass of the jth unmixed gas parcel at combustor end to the cumulative mass of the jth unmixed gas parcel at the PZ1 end
$f_{j,pz1e}$	the ratio of the cumulative mass of the jth unmixed gas parcel at PZ1 end to the cumulative mass of the jth unmixed gas parcel at the PZ1 end (=1)
$f_{j,pz2e}$	the ratio of the cumulative mass of the jth unmixed gas parcel at PZ2 end to the cumulative mass of the jth unmixed gas parcel at the PZ1 end
g	the ratios of the cumulative mass of added DCA at any time to the total DCA mass to be added into the PZH and DZ
g_{ce}	the ratios of the cumulative mass of added DCA at combustor end to the total DCA mass to be added into the PZH and DZ
g_{pz1e}	the ratios of the cumulative mass of added DCA at PZ1 end to the total DCA mass to be added into the PZH and DZ
g_{pz2e}	the ratios of the cumulative mass of added DCA at PZ2 end to the total DCA mass to be added into the PZH and DZ
$m_{cu,ce}$	the cumulative flowed total gas mass at the combustor end during the combustor residence time (kg)
$m_{cu,dca,ce}$	cumulative added DCA mass at the combustor end (kg)
$m_{cu,dca,pz1e}$	cumulative added DCA mass at the PZ1 end (kg)
$m_{cu,dca,pz2e}$	cumulative added DCA mass at the PZ2 end (kg)
$m_{cu,j,ce}$	cumulative mass of jth gas parcel at the combustor end (kg)
$m_{cu,j,pz1e}$	cumulative mass of jth gas parcel at the PZ1 end (kg)
$m_{cu,j,pz2e}$	cumulative mass of jth gas parcel at the PZ2 end (kg)
$m_{cu,j,ce}$	cumulative mass of jth gas parcel at the combustor end (kg)
Δm_{dca}	total DCA mass to be added into the PZH and DZ of the combustor during the PZH and DZ residence time (kg)
N	the number concentration of soot particles in a gas parcel (#/kg-gas)
$N_{j,k}$	the number concentration of soot particles in the kth size bin in the jth gas parcel (#/kg-gas)
N_k	the number concentration of soot particles in the kth size bin at any time (or at any cross section) of the combustor and turbine (#/kg-gas)
n_p	number of unmixed gas parcel
n_{sp}	total number of chemical compounds
n_{st}	total number of soot size bins in sectional aerosol dynamics model
n_{stp}	total number of fuel rich soot gas parcels whose mass fraction change rate through out the combustor were set different than all other gas parcels
$n_{wlp;}$	total number of fuel lean wall region gas parcels whose mass fraction change rate through out the combustor were set different than all other gas parcels
P_{atm}	pressure in the atmosphere (atm)
$P_{ci,idl}$	combustor inlet pressure for idle operating condition (atm)
$RP_{ci,idl\text{-}to}$	the ratio of combustor inlet pressure during idle to that during take-off
$RT_{ci,idl\text{-}to}$	the ratio of combustor inlet temperature during idle to that during take-off
r_{pz1}	the ratio of residence time of the primary zone 1 of the combustor to the residence time of the whole combustor
r_{pzh}	the ratio of residence time of the primary zone hole of the combustor to the residence time of the whole combustor
r_{tn}	the ratio of residence time of the turbine and nozzle to the residence time of the whole combustor
T_{atm}	temperature of the atmosphere (K)
$P_{ci,idl}$	combustor inlet pressure for idle operating condition (atm)
P_{tne}	pressure at the turbine and nozzle exit (atm)
t	cumulative residence time (s)
T	temperature at any time (or at any cross section) of the combustor and turbine (K)
$T_{0,j}$	initial temperature of jth unmixed gas parcel at the start of simulation (at combustor inlet) (K)
T_j	temperature of jth gas parcel (K)
T_{tne}	temperature at the turbine and nozzle exit (K)
Z	the mass fraction of a chemical compound in a gas parcel
$Z_{dca,i}$	the mass fraction of ith chemical compound in DCA
Z_i	the mass fraction of ith chemical compound at any time (or at any cross section) of the combustor and turbine
$Z_{j,i}$	the mass fraction of ith chemical compound in jth gas parcel

Greek letter

α	the ratio of cumulative mass of a gas parcel at any time to the cumulative flowed total gas mass at the combustor end during the combustor residence time