Status of Superheated Spray and Post Combustor Particulate Modeling for NCC

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ABSTRACT
At supersonic cruise conditions, high fuel temperatures, coupled with low pressures in the combustor, create potential for superheated fuel injection leading to shorter fuel jet break-up time and reduced spray penetration. Another issue particularly important to the supersonic cruise is the aircraft emissions contributing to the climate change in the atmosphere. Needless to say, aircraft emissions in general also contribute to the air pollution in the neighborhood of airports. The objectives of the present efforts are to establish baseline for prediction methods and experimental data for (a) liquid fuel atomization and vaporization at superheated conditions and (b) particle sampling systems and laboratory or engine testing environments, as well as to document current capabilities and identify gaps for future research.
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Relationship to the Fundamental Aeronautics Program

- **Project**: Supersonic
- **Discipline**: High Altitude Emissions
- **Element**: Emissions Prediction and Modeling
- **Tasks**
  - Superheated atomization and vaporization modeling
  - Particle chemical and microphysics modeling
Atomization and Vaporization Models at Superheated Conditions (SUP 1.04.02)

Background

At supersonic cruise conditions, high fuel temperatures, coupled with low pressures in the combustor, create potential for superheated fuel injection leading to shorter fuel jet break-up time and reduced spray penetration. In several scramjet and ramjet engine conditions, flash injection occurs when there is a rapid pressure drop through injection to a pressure well below the saturation pressure of the liquid.
Atomization and Vaporization Models at Superheated Conditions (SUP 1.04.02)

Objectives

Establish baseline for prediction methods and experimental data for liquid fuel atomization and vaporization at superheated conditions.

Document current capabilities and identify gaps for future research.

Ultimate goal is to improve prediction capabilities for emissions and performance at supersonic cruise conditions using Combustion CFD simulations.
Approach

Modify the atomization models to account for the flash boiling effects on the primary breakup.

Incorporate superheated vaporization models for fuel droplet transport.

Conduct literature survey to gather experimental data suitable for model validation.

Perform validation calculations and assess the current status of models and experimental data.
Milestone Status (SUP 1.04.02)

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<td>Integration of atomization model, superheated vaporization model into NCC version 1.1.8</td>
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<td>Collect and assess available superheated experimental data</td>
<td>5/2007</td>
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<td>Perform calculations using NCC and compare with data</td>
<td>10/2007</td>
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**Major Issues**

The quantitative fidelity of the existing models at superheated conditions has not been well documented in the open literature. Validation data are very sparse and limited in terms of fuel type and injection environment.
Experimental Investigation of Superheated Liquid Jet: Atomization due to Flashing Phenomena
(Yildiz et al. (2005), VKI FLIE Seminar, Milan – 2005)

Material: Refrigerant R134A (at 1 atm, the boiling temperature is -26.7 C, i.e., 246.3K)

Nozzle diameter : 1mm
Modeling and Simulation

- Atomization process is not yet simulated, computation was performed by making use of a single-point droplet injection with a solid cone angle of 7.5 degree and a Sauter Mean Diameter (SMD) of 70 microns. It made use of five different droplet groups based on a known droplet correlation. The initial liquid velocity is about 34 m/s and the initial liquid temperature is 260 degree K.
- The whole range drop vaporization model switches from the one for the superheated condition to the one for the normal condition, when the droplet temperature reaches near the boiling temperature.
- At the superheated condition, the model accounts for both the drop flash vaporization and the external heat transfer vaporization.
Experimental and liquid predicted values for temperature over axial distance.

Centerline axial temperature variation for a 1 mm VKI nozzle (Combined superheat-normal vaporization model).

Predicted global structure of a vaporizing spray for a 1 mm VKI nozzle (Combined superheat-normal vaporization model).
Future Plan

• Improve droplet vaporization model and atomization model at superheated conditions.
• Integrate advanced models developed by NRA partners into NCC.
• Acquire experimental data of jet fuel injection under superheated conditions.
• Perform simulations and compare with experimental data.
Chemical and Microphysical Particulate Models (SUP 1.04.04)

Background

Aircraft emissions contribute to climate change in the atmosphere and air pollution in the neighborhood of airports. Assessment of their environmental impacts calls for a better understanding of the formation and the subsequent development of gaseous pollutants, aerosols (volatile particles and soot), and their precursors in the internal flow and in the plume of the jet engines operating over the full range from ground to flight altitude. This is best achieved by the combined use of measurement and modeling studies.
Objective

Establish baseline for prediction methods and experimental data for particle sampling systems and laboratory or engine testing environments.

Document current capabilities and identify gaps for future research.

Ultimate goal is to improve prediction capabilities for particulate emissions at supersonic cruise conditions as well as to assist the development of sampling and measurement methodology for particle emissions.
Chemical and Microphysical Particulate Models (SUP 1.04.04)

Approach

Incorporate finite rate kinetic models for conditions intermediate between combustion and atmospheric chemistry.

Incorporate models for particle microphysics most relevant to aircraft emissions.

Conduct literature survey to gather experimental data suitable for model validation.

Perform validation calculations and assess the current status of models and experimental data.
Milestone Status (SUP 1.04.04)

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<td>Integration of chemical and microphysical particulate models into NCC version 1.1.8</td>
<td>9/2007</td>
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**Major Issues**

The quantitative fidelity of the existing models for aircraft particulate emissions has not been well documented in the open literature.

The repeatable and accurate measurements are challenging due to particle’s sensitivities to sampling system design and ambient conditions.
Current Models

• Particle transport equations are based on the multiple-bin Eulerian approach.
• Models include sulfate and nitrate aerosol precursors, thermophoresis, coagulation, nucleation, soot activation, condensation/evaporation, and interaction between the gaseous species and the particles.
• CFD-based simulation integrates fluid dynamics, chemistry, and particle microphysics.
• Lower-order spatial simulation investigates flow, chemistry, and particle microphysics in the quasi-1D framework.
• Lower-order temporal simulation is one in which chemistry and particle microphysics are driven by averaged flow parameters specified as a function of time.
APEX-3 Particle loss in a sampling line
Anderson et al. (2006)

System was carefully leak-checked to minimize stray particle counts to allow going to high sample dilutions/flow rates.

System flow was adjusted to simulate actual sampling conditions and to evaluate losses as a function of flow rate.

Particle instruments were tested side-by-side prior to experiment to determine any differences in size sensitivity or response.
APEX-3 Particle loss in a sampling line

- Arc length of the first segment of the sampling line is 9.5 m.
- Inside diameter is 0.009525 m (3/8 in).
- Arc length of the second segment of the sampling line is 14 m.
- Inside diameter is 0.019050 m (3/4 in).
- Total length is 23.5 m.
- Flow rate is 50 LPM (11.7 m/s).
- Temperature of the carrier gas is 295 K.
- Upstream pressure is 740 Torr (98627.2 Pa).
- Downstream pressure is 690 Torr (91963.2 Pa).
- Temperature of the wall is 295 K.
- Penetration = $\frac{N_{\text{out}}}{N_{\text{in}}}$
Modeling and Simulation

- CFD-based simulation
  flow is assumed to be axisymmetric.
  particle deposition on the wall is accounted for by the
  assumed gradient of particle number density at
  the wall.
- Lower-order spatial simulation
  empirical correlations are employed to account
  for the viscous effects as well as the particle loss due to
  diffusion and thermophoretic force in pipe flows.
- Lower-order temporal simulation
  velocity, temperature, and pressure are prescribed
  by using Shapiro’s simple flow model.
  empirical correlations are employed to account
  for the viscous effects as well as the particle loss due to
  diffusion and thermophoretic force in pipe flows.
APEX3 line loss (Monodisperse aerosol source)

T=295K, Pupstream=740 Torr, Pdownstream=690 Torr, Flow=50 lpm(11.7 m/s)
First segment: id=0.009525 m (3/8 in), length = 9.5 m
Second segment: id=0.019050 m (3/4 in), length = 14 m

- low-order model - temporal approach
- lower-order model - spatial approach
- CFD-based (area averaged)
First segment: \( \text{id}=0.009525 \text{ m (3/8 in)} \), \( \text{length}=9.5 \text{ m} \)
Second segment: \( \text{id}=0.019050 \text{ m (3/4 in)} \), \( \text{length}=14 \text{ m} \)
First segment: id=0.009525 m (3/8 in), length= 9.5 m
Second segment: id=0.019050 m (3/4 in) length= 14. m

- Low-order model - temporal approach
- Lower-order model - spatial approach
- CFD based (area averaged)
Future Plan

• Improve chemical and microphysical models for aircraft particulate emissions.
• Integrate advanced models developed by NRA partners into NCC.
• Acquire experimental data for particle sampling systems and laboratory or engine testing environments.
• Perform simulations and compare with experimental data.