



The impact of flow features on formation of surface carbonaceous deposits under aero engine representative conditions

E. Alborzi

The University of Sheffield Aviation Fuel Research Fellow Department of Mechanical Engineering, The University of Sheffield, Sheffield, S1 3JD, UK e.alborzi@sheffield.ac.uk

S. Blakey The University of Sheffield Senior Lecturer Department of Mechanical Engineering, The University of Sheffield, Sheffield, S1 3JD, UK

P. Gadsby The University of Sheffield Senior Lecturer Department of Mechanical Engineering, The University of Sheffield, Sheffield, S1 3JD, UK

ABSTRACT

The application of aviation fuel as a heat sink in advanced aircraft propulsion system is an attractive option for the integrated management of the cooling and heating requirements. The use of fuel as a heat sink is however limited by its thermal stability or its propensity to form surface carbonaceous deposits as it is heated. Improved understanding of the flow effects on deposit formation is significant for the staged combustion systems proposed in the next generation of engines particularly around the Reynolds number in transition region where the available literature seems to differ in its assessment of any affect. The impact of different flow features on surface carbonaceous deposit formation was investigated experimentally in an engine representative condition using "Aviation Fuel Thermal Stability test Unit (AFTSTU)" for two sets of simulated burner feed arms including cylindrical structure and contraction/expansion nozzle respectively. Transient CFD models with a two stage kinetic model of surface deposition were used to predict the growth of deposits layer at the inner surface of fuel wetted surface. The simulated results were in good agreement with the experiments.

KEYWORDS: Aviation fuel thermal oxidative stability, Surface deposition, Aero engine

1 INTRODUCTION

The application of aviation fuel as a heat sink in advanced aircraft propulsion systems is an attractive option for the integrated management of the cooling and heating requirements. The use of fuel as a heat sink is however constrained by its thermal stability, or it's propensity to form deposits as it is heated. Improved understanding of the flow effects on this deposit formation is significant for the staged combustion systems proposed in the next generation of engines, specifically on the effects of static fuel autoxidation, where the available literature seems to differ in its assessment of any effect.

Due to its significance as a limiting factor in fuel system design, it is very desirable to create appropriate models capable of predicting various features of thermal degradation for a broad range of conditions and geometries similar to those encountered in real jet fuel system. Accordingly, CFD based models incorporating a realistic physico-chemistry model and validated against suitable experimental data offer the potential of being applicable in the preliminary stage of aircraft fuel system components design. The consistency of CFD models is, however, restricted to a number of parameters including the robustness of physico-chemistry model together with many others such as





the computational techniques applied for the solution of mathematical models, selection of the boundary conditions and etc.

Construction of a physico-chemical model for thermal stability has been a research topic for both fuel producers and jet engine manufacturers. Many aspects of this problem have been established over recent decades; however there are still numerous uncertainties. The sequence of liquid-phase reactions occurring in the course of surface thermal degradation and surface deposition is not very well understood. This is primarily due to the fact that the fuel composition is very complex and the resulting degradation products are numerous. In this regard, chemical analysis and characterization of insoluble materials and deposits found in fuel tanks and aircraft systems indicate that sulfur, nitrogen, and oxygen atoms are highly concentrated in the deposits, strongly supporting their importance in the insoluble/deposit formation processes.[1]

Thermal decomposition of fuel is governed by a number of parameters including chemical composition of fuel(bulk species as well as heteroatomic molecules), bulk fuel and surface temperature, duration of thermal exposure, flow regime of fuel inside the fuel lines and catalytic characteristics of fuel lines surfaces. Concerning fuel chemical composition, it is commonly known that the presence of trace levels of heteroatomic species in jet fuel is known to be a primary contributor to the thermal oxidative instability reactions which are leading to surface deposits formation. Concentration of the heteroatomic species varies largely from one fuel sample to the next. Therefore, any quantitative analysis of fuel thermal stability requires a comprehensive measurement of the heteroatomic species.

Zabarnick [2] and Zabarnick et al.[3] and Kuprowicz et al.[4] proposed a pseudo detailed chemical kinetic mechanism for liquid phase of oxidation of conventional aviation fuels as shown in Table 1. Kinetic parameters of this mechanism have been put together based on a combination of theory, experiment, and trial and error. The surface deposition model is added to the mechanism as a global scheme, with a constant reaction rate, based on the conversion of precursor (insoluble products) to deposit. Incorporated to CFD, such a scheme has had a degree of success in predicting the autoxidation process as well as the surface deposition profiles, for a range of conventional jet fuels and mild conditions in simplified geometries. However, same chemical kinetic mechanism falls short of being applicable for prediction of evolution of surface deposition in engine representative conditions where fluid flow regime and heat transfer characteristics are quite complicated.

From the chemical kinetics point of view, increasing the residence time of thermally stressed jet fuel in heated tubes would be expected to boost the total quantity of carbon deposit, however, it has been shown by Marteneny and Spadaccini, Chin and Lefebvre that the total amount of carbon deposit changes in an inversely proportional trend with respect to the Reynolds number modification for the same diameter of the tube. A possible explanation for such an ambiguous observation is to consider that the increase of radial diffusion acts as a controlling factor for the migration of the deposit precursors (insoluble species).

We have studied the formation of surface deposits at the inner surface of two simulated burner feed arms including a cylindrical pipe and a nozzle with contraction/expansion structure under aero engine representative conditions provided by the "Aviation Fuel Thermal Stability Test Unit (AFTSTU)". A comprehensive description of the AFTSTU, nozzles' configuration and test conditions are given in Alborzi et al. [5] Although the inlet Reynolds number for two simulated burner feed arms is the same the flow feature and heat transfer characteristics for the contraction/expansion nozzle is substantially different from cylindrical nozzle. While flow feature in the cylindrical nozzle is described by a typical fully developed flow, the contraction/expansion burner feed arm presents features such as strong recirculation zones, stagnant flow regions, fully developed and vena contracta which collectively have strong effect on the formation of surface deposits.





Table 1: Pseudo detailed chemical kinetic mechanism for liquid phase of oxidation of jet fuels

| | Reaction | A[mol,L,s] | Ea[kcal/mol] | | Reaction | A[mol,L,s] | Ea[kcal/mol] |
|---|---|--------------------|--------------|----|---|--------------------|--------------|
| 1 | I→R⁺ | 1×10 ⁻³ | 0 | 10 | RO⁺+RH→ROH+ R⁺ | 3×10 ⁹ | 10 |
| 2 | $R^{\bullet}_{+}O_2 \rightarrow RO_2^{\bullet}$ | 3×10 ⁹ | 0 | 11 | $RO^{\bullet} \rightarrow Rprime + Carbonyl$ | 1×10 ¹⁶ | 15 |
| 3 | RO_2 + $RH \rightarrow RO_2H + R$ | 3×10 ⁹ | 12 | 12 | $OH^{\bullet}+RH \rightarrow H_2O+R^{\bullet}$ | 3×10 ⁹ | 10 |
| 4 | RO_2^{\bullet} + RO_2^{\bullet} →termination | 3×10 ⁹ | 0 | 13 | $RO^{\bullet} + RO^{\bullet} \rightarrow RO_{term}$ | 3×10 ⁹ | 0 |
| 5 | $RO_2^{\bullet} + AH \rightarrow RO_2H + A^{\bullet}$ | 3×10 ⁹ | 5 | 14 | $Rprime + RH \rightarrow alkane + R^{\bullet}$ | 3×10 ⁹ | 10 |
| 6 | A⁺+RH→AH+ R⁺ | 1×10 ⁵ | 12 | 15 | $RO_2H+SH \rightarrow Product_{SH}$ | 3×10 ⁹ | 18 |
| 7 | $A^{+} RO_{2}^{-} \rightarrow Products_{AH}$ | 3×10 ⁹ | 0 | 16 | $RO_2^{\bullet} \rightarrow R^{\bullet}_+O_2$ | 1×10 ¹⁶ | 19 |
| 8 | $R^{\bullet} + R^{\bullet} \rightarrow R_2$ | 3×10 ⁹ | 0 | 17 | RO_2 + R · \rightarrow termination | 3×10 ⁹ | 0 |
| 9 | RO ₂ H→RO [•] +OH [•] | 1×10 ¹⁵ | 39 | 18 | $RO_2H+M\rightarrow RO^{\bullet}+OH^{\bullet}+M$ | 3×10 ¹⁰ | 15 |

2 EXPERIMENTAL METHODS

2.1 Description of AFTSTU and test conditions

The AFTSTU is a pilot scale experimental unit capable of assessing the interaction of a simulated engine fuel system and a representative fuel. The AFTSTU simulates conditions in a range of current and future aero engines ensuring that the fuel arrives at a simplified burner feed arm in a representative condition to that in service, which is critical in assessing the likely interaction with hot surfaces and flowing fuel. A simplified schematic the AFTSTU is shown in **Figure 1**. Inside the rig, the thermal regimes from the fuel tank to the burner feed arm are replicated in a modular fashion, allowing for independent control of the heat loading within the various sections of the rig. A representative Jet A-1 fuel was tested in three experiments with AFTSTU. The composition of major hydrocarbon constituents and some of the heteroatomic species along with the corresponding quantification methods are presented in Table 3. Details about the quantification methods are found in Alborzi et al.[5]

Two tests were carried out to study the formation of surface carbonaceous deposits in simulated burner feed arms with cylindrical structure and the contraction/expansion nozzle respectively. The detailed design of both burners feed arm geometries are presented in Figure 2. Three (for cylindrical burner feed arm) and five pairs(for contraction/expansion burner feed arm) of K-type sheathed thermocouples were silver brazed into the wall of the tubes. The outer thermocouples were 0.2mm from the outer tube surface while the inner thermocouples were 0.4mm distant from the inner tube surface. The test parameters used in the AFTSTU are illustrated in Table 2. A "Radio Frequency (RF)" induction heating coil with a total length of 120mm was centred on the central pair of thermocouples. Induction heating is mostly a skin effect where electromagnetic field is only present in the first millimeters of the heated specimen. Therefore, at the operating frequency of the heater around 280 KHz, 87% of the power was dissipated in less than the first 0.6mm of the outer surface.

| Test condition | Values | | |
|---------------------------------------|--------|--|--|
| Test time (hrs) | 75 | | |
| Fuel flow rate (L/hr) | 23 | | |
| Low pressure system (psi) | 50 | | |
| LP bulk fuel temp (°C) | 50 | | |
| LP cabinet (°C) | 50 | | |
| High pressure system (psi) | 500 | | |
| HP bulk fuel temp (°C) | 180 | | |
| HP cabinet (°C) | 180 | | |
| Time (hrs) | 25 | | |
| Bulk fuel temp rise along nozzle (°C) | 18 | | |

Table 2: AFTSTU test parameters



Figure 1 : Simplified schematic of the AFTSTU rig modules

| Chemical species | Concentration | Unit | Method |
|----------------------|---------------|-------|---|
| n-Paraffins | 20.67 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Iso-Paraffins | 24.77 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Cyclics | 30.84 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Alkeylbenzenes | 16.18 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Indans and teralins | 2.15 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Naphtalenes | 1.33 | % m/m | CMS- 269985 by GC X GC- FID(UOP990) |
| Antioxidants | 25 | mg/l | CMS- 269985 by GC X GC- FID(UOP990) |
| Thiols and sulfides | 210 | mg/Kg | CMS- 269985 by GC X GC- FID(UOP990) |
| Total hydroperoxides | 4.7 | μM | West et al.[6] |
| Dissolved metals | 52 | mg/Kg | MT/ELE/15 |
| Dissolved oxygen | 70 | ppm | Value from the references [2][3][4] [7] |

| | Table 3: Chemical | composition | of Jet A-1 | fuel and | test methods |
|--|--------------------------|-------------|------------|----------|--------------|
|--|--------------------------|-------------|------------|----------|--------------|



Figure 2: Schematic drawings of two simulated burner feed arms ((not to scale, dimensions in mm)





3 DESCRIPTION OF SURFACE DEPOSITION MODEL

The two stage kinetic transient model is described in equations 1-6. The model presents an explicit way for calculation of cumulative surface deposition rate. This method is partly based of works published by Ervin et al.[8], Katta et al.[9] and Roquemore and Reddy[10]. We proposed an additional equation that accounts for the cumulative rate of deposition purely based on experimental results of different types of aviation fuels obtained in our lab. It is noteworthy that due to the large number of complexities associated with the fuel-wetted surface and surface interactions, an exponent n as a calibrating parameter is used in (5 to tune the model. The proposed model needs to be expanded in order to explain the physico-chemical interactions of the surface deposition. The existing model found in the public literature considers one step reaction for conversion of insoluble materials to deposits. We have included one more steps to be able to simulate the non-linear formation of deposits over time.

$$\left[\frac{d\delta}{dt}\right]_{t=0} = k_1 \left[\frac{\rho_{insoluble} f_{insoluble}}{MW_{insoluble}}\right]$$
(1)

$$k_1 = A_1 e^{\left(\frac{-Ea_1}{RT}\right)} \tag{2}$$

$$\Delta\delta = r - r_0 \tag{3}$$

$$r = r_0 \sqrt{1 - \frac{2\left(\frac{d\delta}{dt}\right)_{t+\Delta t}}{\rho_D r_0}}$$
(4)

$$\left[\frac{d\delta}{dt}\right]_{t+\Delta t} = k_2 \left(\frac{\Delta\delta}{r_0}\right)^n \tag{5}$$

$$k_2 = A_2 e^{\left(\frac{-Ea_1}{RT}\right)} \tag{6}$$

Due to the large number of complex molecular interactions at fuel-surface interface, construction of a detailed model capable of capturing all of the physico-chemical interactions in the course of fuel deposition is extremely challenging. Epstein[11] assumed that the arrival of the insoluble species at a surface can occur by two mechanisms including gravitational settlement and particle transport. It is believed that the gravity effect may be negligible as radial diffusion in bulk fuel is vigorous. A combination of turbulent diffusion and Brownian motion must drive the precursor at the surface. The small size particles obey the Brownian and eddy diffusion while the large particles move according to momentum forces due to their greater mass. Another possibility for surface deposit formation is to





assume that the deposit particles are initiated at the heated surface with little contribution form particles in the bulk fuel. The third possibility is that the surface deposition results from the contributions of both adhering bulk particles and deposits formed at the wall.

The third possibility can be justified with the assumption made by Moses[12] that when the temperature at fuel wetted surface is at least 45°C higher than core temperature, almost 90% of the insoluble materials will be formed within the laminar sublayer. This justification is based on the fact that approximately two thirds of temperature change occurs within the laminar sub layer and that the formation of deposit precursors follows an exponential relation to bulk fuel temperature.

Regardless of the precursor migration to the wall, there are a multitude of complex physical interactions which can take place for deposition to occur. These processes can be highlighted as:

- The agglomeration of insoluble oxidation product molecules in jet fuel to micro spherical particles 500-3000 Å
- Collection, through which the micro spherical particles settle on the surface of bulk fuel or collect on the surface after impingement from the moving fluid. Meanwhile, the more volatile species can leave the surface, and in that case heavier species may remain
- Surface Fusion, during which particles may experience coalescence and plastic flow type to form varnish like substrate upon which additional particles collect. Further oxidation may occur to form coke like deposits.

The temperature regime plays a significant role on thermal oxidative chemical reactions. The temperature increases the rate of the autoxidative reactions. The dependency of single step reaction to the temperature is relatively easy when the kinetic expression is known for the reaction, for instance, zero order kinetic, first order and etc. However, the situation is different in the case of chain reaction. This is due to the fact that the change in temperature not only changes the rate of reaction steps but can change the mechanism of the reaction and composition of the formed products.

The computational domains for CFD simulation are shown in Figure 3. Steady state calculations were performed to predict the temperature profile along the inner surface prior to the fuel thermal exposure. The boundary conditions are specified in such a way that the fluent model can accurately predict the behavior of the fuel flow field and heat transfer across the tube wall. The inlet velocity boundary condition was applied to the fluid inlet for a location > 12D prior to the physical fuel inlet. Both velocity magnitude and temperature becomes fully developed prior to the physical fuel inlet. In addition, a turbulent intensity of 5% and hydraulic diameter of 2mm for the cylindrical burner feed arm and 0.78 mm for contraction/expansion nozzle were used. A wall boundary condition was applied to the wall inlet, and outlet and outer wall. A zero-heat flux was set up for the thermal condition on both the wall inlet and outlet. As far as the outer wall outlet was concerned, heat flux was specified in equation: **Simplified schematic of the AFTSTU rig modules** (7).

$$Q = h(T_a - T_w) + \varepsilon \sigma (T_a^4 - T_w^4)$$

(7)

Where the external emissivity, ϵ is 0.4 for most types of steel[13], and the free stream temperature, T_a , = 298K. The outer tube wall temperature alongside the tube, T_w is unknown, hence a UDF was written to extract the temperatures from each cell at the outer wall of the tube. The external natural convection heat transfer coefficient was calculated to be 13.94 W/m²K. The inner tube wall is defined by a coupled wall boundary condition, where a no slip condition is applied and based on choice of the turbulence model, the wall roughness height is adjusted accordingly. The exit of the tube is defined as an outflow boundary condition, due to the unknown velocity and pressure field at the outlet. K- ϵ turbulence model with enhanced wall function was used for cylindrical tube. Due to the complexity of flow and heat transfer in the contraction/expansion burner feed arm, more accurate results were obtained when k- ω model with finer mesh in proximity of the heated wall was used. Once the steady





Aerospace Europe **6th CEAS Conference**

state calculations were performed accurately, the surface deposition model was applied to the boundary corresponding to the fuel wetted surface. In order to do this, a UDF was created. The local values of molar concentration of insoluble were calculated based on the pseudo detailed mechanism shown in Table 1. The chemical species boundary conditions were taken from work published by Kuprowicz et al. The computational domains are shown in Figure 3.



Figure 3: Computational domains for CFD simulation

4 **RESULTS AND DISCUSSION**

The results shown in Figure 4 : Simulated temperature profiles at the fuel wetted surfaces for cylindrical burner feed arm (left) and burner feed arm with contraction expansion (right) indicate good agreement between measurements and simulated temperature profiles for both burner feed arm. This is an important point at the accuracy of simulated deposit depends upon the precision of temperature profile at the fuel wetted surfaces prior to the fuel thermal stress. For the case of contraction/expansion nozzle, more accurate results was achieved by the use of $k-\omega$ turbulence model with enhanced wall function with finer mesh in the regions where mixing and flow separation were pronounced as shown in Figure 5. The complex flow features including strong mixing zone at the corners of expansion and contraction regions as well as the flow separation and re attachment influence the heat transfer before and after the expansion and contraction. This result in two regions of temperature drop after the step change due to the decrease of heat transfer coefficient.

Formation of surface deposits is associated with the increase of temperature at the outer surface of burner feed arms. The reason for temperature rise is due to the formation of an insulative layer composed of carbonaceous with substantially lower thermal conductivity in comparison to the stainless steel. A mathematical model for calculation of deposit thickness from temperature rise data is given in Alborzi et al[5] and Alborzi et al[14](currently under review).

The results of transient CFD simulations for prediction of local deposit thickness at thermocouple's tips for both burner feed arms are shown in Figure 6 and Figure 7. The simulated results are in good agreement with the measurements. Due to the strong mixing regions, residence time at the flow stagnant regions increase substantially. This results in considerably higher amount of total deposits at burner feed arm with contraction/expansion structure in comparison to the nozzle with cylindrical structure.







Figure 4 : Simulated temperature profiles at the fuel wetted surfaces for cylindrical burner feed arm (left) and burner feed arm with contraction expansion (right)



Figure5: Contour of streamlines along the heated nozzle including expansion/contraction geometry after expansion (left), Contour of streamlines showing formation of vena contracta after tube contraction. Both pictures were enlarged in radial direction for clear graphical presentation), see Alborzi et al.[5]



Figure 6: Predicted deposit thickness along the heated surface (left) and vs time at first thermouple's tip (right) for burner feed arm with cylindrical structure



Figure 7 : Predicted deposit thickness along the heated surface (left) and vs time at fourth thermouple's tip (right) for burner feed arm with contraction/expansion structure

5 CONCLUSIONS

- A new sub model for the deposition step of the thermal stability deposit formation process has been proposed and successfully validated against to nozzles under engine representative conditions provided by the AFTSTU
- The validated deposition sub model demonstrates the importance of the heat transfer boundary conditions on the modelling of thermal stability deposition
- The formation of complex flow features including stagnant flow regions, reattachment and vena contracta has a strong impact on total mass of deposits form in the nozzle.





REFERENCES

1. R.N. Hazlett, 1991; "*Thermal Oxidation Stability of Aviation Turbine Fuels*", , CRC. 1991.

2. S. Zabarnick, Chemical Kinetic Modeling of Jet Fuel Autoxidation and Antioxidant Chemistry, Industrial & Engineering Chemistry Research, 32, 1993, 1012–101.

3. S. Zabarnick, Pseudo-Detailed Chemical Kinetic Modeling of Antioxidant Chemistry for Jet Fuel Applications , (97), 1998, 547–553.

4. N. J. Kuprowicz, S. Zabarnick, Z. J. West, J. S. Ervin, T. Edwards, Use of Measured Species Class Concentrations With Chemical Kinetic Modelling for the Prediction of Autoxidation and Deposition of Jet Fuels, Energy & Fuels, 2007, 530–544.

5. E. Alborzi, S. Blakey, H. Ghadbeigi, C. Pinna, C. Lewis, Investigation of surface deposition in a simulated fuel injector feed arm with sudden expansion/contraction, Fuel, 186, 2016, 534–543.

6. Z. J. West, S. Zabarnick, R. C. Striebich, Determination of Hydroperoxides in Jet Fuel via Reaction with Triphenylphosphine, Industrial & Engineering Chemistry Research, 44, 10, 2005, 3377–3383.

7. D. Boss, R. N. Hazlett, R. L. Shepard, Analysis of n-Paraffin Oxidation Products in the Presence of Hydroperoxides, Analytical chemistry, 45, 14, 1973, 14–18.

8. J. S. Ervin, S. Zabarnick, T. F. Williams, One-Dimensional Simulations of Jet Fuel Thermal-Oxidative Degradation and Deposit Formation Within Cylindrical, Journal of Energy Resources Technology, 2002, 229–238.

9. V. R. Katta, R. W. M, Numerical Method for Simulating Fluid-Dynamic and Heat Transfer Changes in Jet Engine Injector Feed Arm Due to Fouling, Journal of Themophysics and Heat Transfer, 7, 1993, 651–661

10. W. M. Roquemore, K. V. Reddy, A Time Dependent Model with Global Chemistry for Decomposition and Deposition of Aircraft Fuels, in: Symposium on the Stability and Oxidation Chemistry of Middle Distillate Fuels, 1990, pp. 1346–1357.

11. Epstein N, Particulate Fouling of Heat Transfer Surfaces: Mechanisms and Models. In: Mel1988) o L.F., Bott T.R., Bernardo C.A. (1988) Fouling Science and Technology. NATO ASI Series (Series E: Applied Sciences), vol 145, 1988 Springer, Dordrecht

12. C. Moses and G. Wilson, Studies of the Kinetics of Jet Fuel Thermal Stability By Laser Induced Fluorescence, IASH 2007, the 10th International Conference on Stability, Handling and Use of Liquid Fuels, Tucson, Arizona, October 5-11, 2007

13. Incropera, F P. and David, P Dewitt. and Theodore, L Bergman. And Adrienne, S Lavine , Introduction to Heat Transfer, 5th Edition, Wiley, 2005

14. E. Alborzi , S. Blakey, H. Ghadbeigi, C. Pinna, Prediction of Growth of Jet Fuel Autoxidative Deposits at Inner Surface of a Replicated Jet Engine Burner Feed Arm, Journal of Fuel(2017)(Under review)