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**A TIME-DEPENDENT MODEL WITH GLOBAL CHEMISTRY
FOR DECOMPOSITION AND DEPOSITION OF AIRCRAFT FUELS**

By

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Abstract

The complicated decomposition processes of a thermally stressed aircraft fuel are mathematically treated using a computational fluid dynamics (CFD) base model with global chemistry. Recently Krazinski et al. (6) proposed a time-averaged CFD model with global chemistry for predicting the deposition rate of jet fuel. This model has proven to give reasonable results when calculations are compared to heated tube experiments lasting 25 hours or less. However, longer duration heated tube experiments have shown that the deposition rate increases with test time. This cannot be adequately treated by the time-average model since it assumes that the deposition rate is independent of time. This paper presents a time-dependent CFD model with global chemistry that directly accounts for deposit build-up and the impact this has on the fuel velocity and heat transfer rate and, thus their effect on deposition rate. The time-dependent incompressible Navier-Stokes equations along with the species continuity and energy equations are solved in an uncoupled manner using a fully implicit scheme. The model uses the global chemistry model proposed by Krazinski et al., but also assumes that the surface deposition reaction rate increases as a power of the deposit thickness. Comparisons of predictions with data from long duration tests, show that the model gives reasonable results for test durations of 150 hours or less but begins to deviate substantially for longer test times. Future improvements to the chemistry in the model are needed to correctly account for the effects of very long test times on deposition rate.

Introduction

The thermal stability of future jet fuels and the processes that result in fouling of fuel system components are of increasing concern. Thermal stability refers to the potential of a fuel to thermally decompose into insoluble products that can adhere to solid surfaces. Exceeding the thermal stability limit of a fuel in an aircraft fuel system can result in sticking of fuel control valves, poor performance of heat exchangers, clogging of fuel nozzles and hot streaks in the combustor due to an alteration of fuel nozzle spray pattern (1). Although these fouling problems occur sporadically in today's engines, they are expected to be more serious in future high performance aircraft due to the higher heat loads that the fuel will experience as it is used to cool the engine lube oil, avionics, environmental systems, and the fuel controls (2).

The thermal stability of jet fuels has been studied for many years. Quality control methods and empirical design information for hot fuel system components such as heat exchangers and fuel nozzles have resulted from these studies (1). Also, a considerable quantity of data have been collected for different experimental conditions and test apparatus. However, the overall complexity and a lack of fundamental understanding of the processes leading to fouling has hindered the development of a general theoretical framework that can be used to interpret or predict different experimental results. Two empirically based fouling models with similar global kinetics for fuel decomposition chemistry have been developed (3,4). One of the models (4) contains heat and mass transport expressions, which makes it potentially applicable to many engineering problems. However, the empirically based models do not provide, in a fundamental way, the general mathematical framework necessary for predicting the thermal deposition of different jet fuels for radically different experimental apparatus with a wide range of operating conditions. Thus, they do not have the general theoretical framework needed to interpret and predict the results for many different types of experiments. On the other hand, recently proposed computational fluid dynamics based models with global chemistry (CFDC) (5,6) do have the potential of being generally applicable for different test section geometries and a wide range of test conditions. Furthermore, the CFDC models can serve as an aid in designing meaningful experiments, interpreting experimental results in terms of fundamental processes, evaluating theories, providing insights into coupled processes, and estimating the relative sensitivity of parameters associated with fouling.

This paper extends the CFDC thermal stability modeling approach by solving the time-dependent Navier-Stokes equations instead of the Reynolds or time-averaged equations as done in Refs. 5 and 6. The model takes into account the build-up of deposits with time and the impact this has on the fluid velocity and heat transfer rate at the fuel/solid interface. The global chemistry model of Krazinski (6) is used in the present analysis along with the preexponential and activation energies determined therein. These global kinetic parameters were determined by curve fitting procedures using data from short duration tests of 25 hours or less.

Effects of Long Duration Testing on Deposition Rate

The importance of time on the deposition rate was demonstrated in long duration tests conducted by Giovanetti and Szetela (4) and Marteny (7). The average deposition rate at 500 hours is a factor of approximately two greater than that at 400 hours and is approximately four times that at 100 hours (7). This increase is larger at lower wall temperatures than at higher wall temperatures. Since clean fuel is always entering the test section, these changes in deposition rate with exposure time suggest that changes in surface reactivity and changes in fluid dynamics and heat transfer due to deposit blockage might be important factors. A microscopic analysis of deposit surfaces revealed that they are highly irregular and granular (7). The surface irregularity and the structure of the cavities depend mainly on the fluid velocity and the deposit thickness. This rough surface might affect the deposit growth rate by trapping fuel in the cavities and altering the surface sticking properties. Because of the constant heat flux used in heating the fuel, the trapped fuel may experience higher temperatures and residence times than the surrounding flowing fuel thereby, yielding more deposits. Blockage of the tube also becomes significant for long duration tests. At a fuel velocity of 0.076 m/s, Marteny (7) observed only a 43 percent open area after 50 hours of testing. This dropped to 16 percent after 150 hours. The blockage is not evenly distributed along the length of the tube because of the way the deposition rate depends on temperature. The large blockage with uneven distribution of deposits alters the fuel velocity and the heat transfer rate which can, in turn, change the deposition rate. These factors are considered in the time-dependent CFDC thermal stability model.

Mathematical Approach

The time dependent Navier-Stokes equations along with the turbulent energy and species conservation equations are used to describe the fuel motion in a long thin circular tube that is heated electrically with a constant heat flux. To advance the calculations with large time steps (to complete the hundreds of hours of real time within a few minutes of computational time), the governing equations are discretized into finite-difference equations and then are integrated using a fully implicit scheme. At each time step, the oxygen and precursor conservation equations are solved simultaneously with the other governing equations in an uncoupled manner.

The present formulation allows the deposit to grow on the wall surface with test time. In other words, after every time step, the geometry of the fuel/deposit interface, is allowed to change as part of the solution procedure. The computational domain is bounded between the axis of symmetry and the fuel-deposit interface and the grid system is reconstructed after every time-step for the changes in the boundary shape.

The mass, momentum and energy transport equations of the governing equations contain several coefficients related to molecular diffusion, viscosity, and thermal conductivity, respectively. Since a wide range of temperatures exists within the test section, the transport properties of the fuel vary significantly. A fresh JP-5 fuel is used as the fluid in the present calculations and the transport properties, along with the enthalpy and density at the given temperature, are obtained from the curve fits, just as done in Ref. 6.

Chemical Kinetics

Although there is only a limited understanding of the thermal decomposition processes in jet fuels, it is widely believed that they involve oxidation and pyrolysis of hydrocarbon fuel molecules and the formation of radical species (8,9). Autoxidation of the fuel, which is promoted by dissolved oxygen, occurs at temperatures up to about 540 K. Krazinski, et al. (6) used a global kinetics model with two reaction steps to account for the autoxidation reaction. This model did well in predicting the deposition rates in different heated tube experiments and is used in the present analysis. The two reaction steps of this model, which are assumed to occur in the bulk fuel, can be written as follows:



Step 1 generates the important deposit forming precursor species through an autoxidation process. The removal of precursors from the deposition process is assumed to occur at higher temperatures through the second reaction step. A wall reaction, that is similar to the oxidation reaction but, with different reaction rate constants, is also used as a surface reaction mechanism.

To take into account the effects of test duration on the wall reaction, the rate constant for the wall autoxidation reaction is assumed to be a function of both temperature and deposit thickness. Experimental observation (7) indicates that the deposition rate, thickness and granularity of the deposits increase with test duration. This suggests that the number of sites on which the deposit can form increases with time. As a first approximation, the wall reaction rate is assumed to be:

$$\text{Reaction Rate} = k (\Delta h/R)^m \exp(-E_a/R_0T) \quad 1)$$

Here, Δh is the deposit thickness at any given axial location on the tube with initial inner radius R , m is a constant to be determined and k is the pre-exponential constant used in Ref. 6. In the above global reaction model, all the precursors produced on the wall surface and those transported from the bulk fuel to the wall, are assumed to stick to the wall instantaneously and form a deposit. After the $(n+1)$ time-step, the deposit thickness is calculated by updating the deposit geometry at the n th time-step using the expression:

$$\Delta h^{n+1} = \Delta h^n + (\Delta t) P / \text{Density of the Deposit} \quad 2)$$

where P is the rate of generation of precursor particles on the wall surface due to the wall reaction and molecular transport mechanisms.

Results

The time-dependent CFDC model was initially evaluated by repeating the CFDC time averaged calculations presented in Ref. 6. Using the same rate boundary conditions and global reaction model, the time-dependent calculations of wall and fuel temperatures, fuel velocity,

turbulent intensities, deposition rate, and concentrations of precursor and oxygen converged to steady-state values that were in agreement with the time-averaged calculations performed using the model in Ref. 6. For this initial check out of the model the influence of deposit growth on the flow field and heat transfer rate, nor the increase of the surface reaction rate with deposit thickness, these capabilities were not activated. This was necessary to simulate the conditions in the time-average CFDC model.

Marteny (7) conducted a series of experiments to investigate the dependence of deposition rate and deposit morphology on test time duration. The fuel was thermally stressed as it flowed through electrically heated stainless steel tubes with an inner radius of 1.08 mm. A constant heat flux along the 914.4 mm tube length was maintained for the duration of a test. Steady-flow test were conducted from 25 to 500 hours. Tests were run at fuel inlet velocities of 0.0762 m/s and 0.3048 m/s. These test results are used to investigate the capabilities of the time-dependent CFDC model. The ability of the model to correctly determine the dependence of deposition rate and deposit thickness on test duration are of prime interest in the following results.

Figure 1 is presented to demonstrate how the deposit thickness and deposition rate change with wall temperature for test durations of 50 and 150 hours and a fuel velocity of 0.0762 m/s. Two types of calculations are presented. Both have $m = 0$ in the surface deposition rate equation (Eq. 1). In one calculation, the influence of deposit blockage on the fluid dynamics and heat transfer processes is not taken into account. In this case, the time-dependent calculations converged to a steady-state solution shown in Fig. 1. In this case the solution is the same as would be obtained by using the time averaged model in Ref. 6. For the steady-state solution, the total deposition rate is the mass of deposit divided by the test time. By using a deposit density of 0.9 g/cc, as recommended in Ref. 7, this linear relationship can be used to calculate the deposit thickness for the two test times. The deposit thickness results are also shown as steady-state solutions in Fig. 1.

The second type of calculation presented in Fig. 1 considers the influence of deposit blockage as a function of time on the fluid dynamics and the heat transfer processes. These calculations show that the deposition rate is not influenced at the low wall temperatures and only weakly influenced at the higher wall temperatures. The model does, however, give the correct trends. The model predicts that the deposition rate should increase more rapidly at the lower wall temperatures than for the higher wall temperatures, and that after 150 hours the deposition rate reaches a saturation value at a wall temperature of about 550 K. These trends are also observed in the experiments. Figure 1 also shows that the predicted deposit thickness is also only weakly

influenced by the effects of blockage on deposit formation. However, there is a significant discrepancy in the two measured thicknesses and the calculated values.

The experimental deposition rates shown in Fig. 1 for the 50 and 150 hours tests have a larger separation than the calculated rates. This indicates that the deposition rate mechanism is different from that used in the model. In Fig. 2, calculations are presented in which the deposition rate in Eq. 1 is assumed to go as the deposit thickness to a power $m = 0.8$. This assumption appears to improve the agreement between the calculated and measured deposition rates as compared to those in Fig. 1. The deposit thicknesses are also in better agreement but the calculated values are lower than the measured values. This is inconsistent with the fact that the calculated deposition rates are consistently higher than the measured values. The deposit thickness appears to be a sensitive function of deposit density. This opinion was reached by repeating the calculations for different deposit densities. It was determined that with a deposit density of 0.15 g/cc, the deposit thickness would agree with the measured values. However, the value of m had to be limited to 0.8 in order to keep deposition rate from becoming unrealistically high. The sensitivity of deposit thickness to density illustrates the importance of having accurate measurements of deposit density.

Calculations have also been made with the same tube but at a higher inlet fuel velocity (0.3048 m/s) and using a value of $m = 0.8$. At this velocity, the flow inside the tube is transitional. Since the present CFDC code can only simulate either a completely laminar or a fully turbulent flow, two calculations are made at this velocity; one with the assumption that the flow is laminar, and the other with a fully turbulent flow assumption. In the heated-tube section, the laminar flow assumption yields more accurate values of wall temperatures but the predicted bulk temperature is very low compared to the experimental data. On the other hand, the overall temperature distribution is better for the turbulent flow simulation and fairly accurate bulk fuel temperatures are obtained; but, agreement for the wall temperatures is poor near the entrance region up to 500 K. These results are shown in Fig. 3. Since the experimental data for deposition rate are available only up to 500 K, laminar flow simulations are used to predict the deposit growth.

The predicted and measured deposition rates are plotted in Fig. 4 for long duration tests with a fuel velocity of 0.3048 m/s. For test durations up to 300 hours, the predicted deposition rate curves closely follow the experimental data. For very long exposure times and low wall temperatures, however, the computed deposition rates are significantly lower than the measured values and at the higher temperatures the deposition rates undergo rapid increases. This trend is not observed in the experimental results.

Summary and Conclusions

A time-dependent CFDC model for predicting the thermal autoxidation decomposition and deposition characteristics has been developed. This model is used to estimate the effects of long duration tests on deposition rate as measured by Marteny (7). The experimental result that the deposition rate increases significantly with time, suggests that the deposition rate depends in some way on the deposits that are already present. It was assumed in the model that the surface deposition rate increases with deposit thickness. This resulted in fair agreement of deposition rates for test times of less than 150 hours but poor agreement for longer times. The calculated deposit thicknesses were also in poor agreement with measured values for the shorter duration tests. In conclusion, additional work must be performed on the model to better account for the effects of test time duration on deposition rate and deposit thickness.

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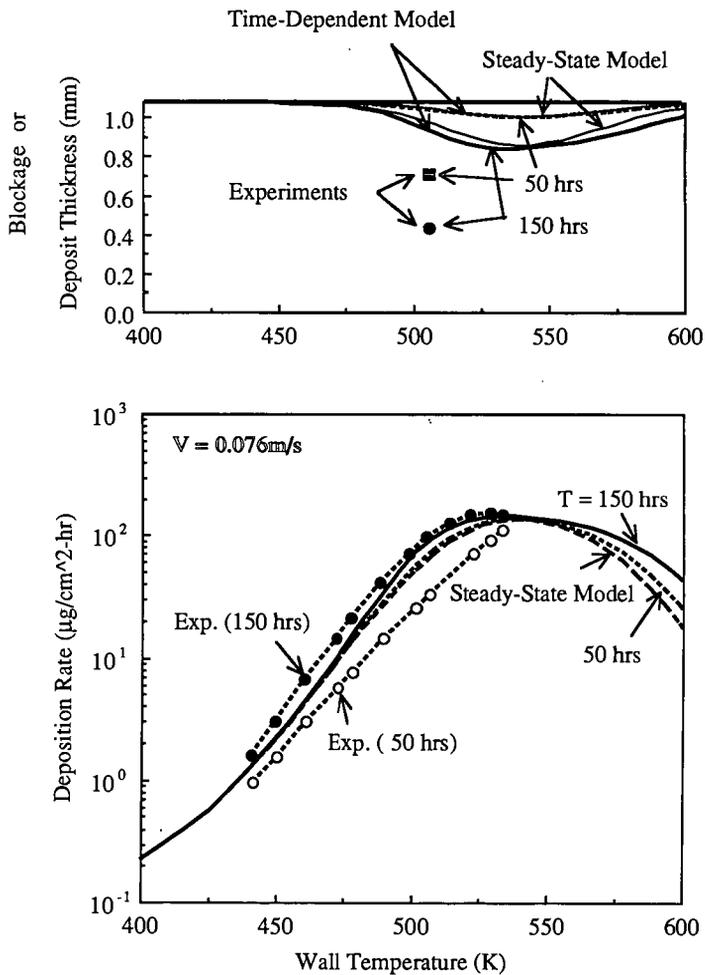


Figure 1. Predicted (without Changing Wall Reaction) and Measured Deposition Rates and Blockages for Long Duration Heated Tube Experiments of Marteny (1989).

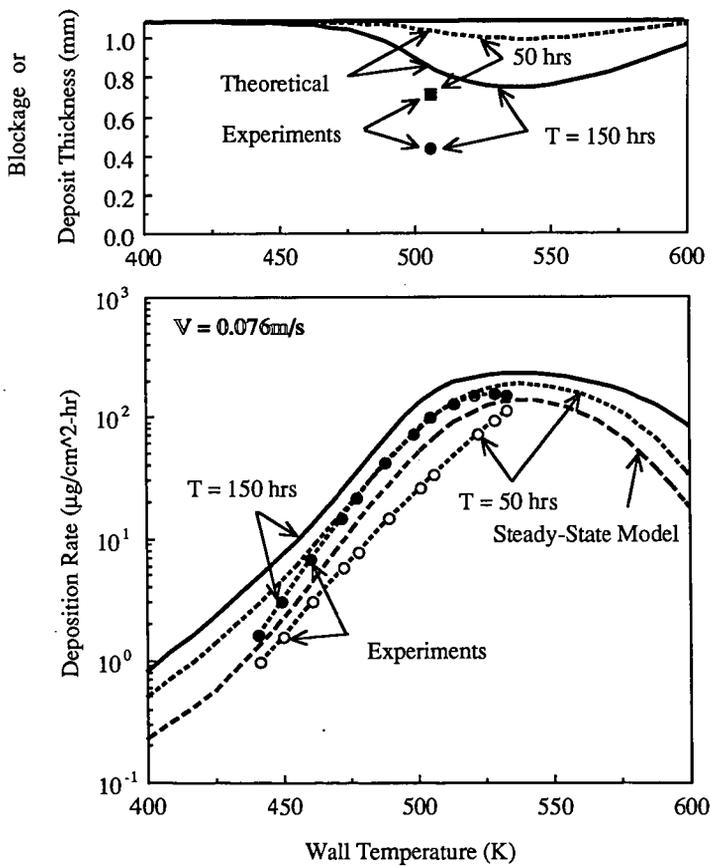


Figure 2. Predicted and Measured Deposition Rates and Blockages for Long Duration Heated Tube Experiments of Marteny (1989).

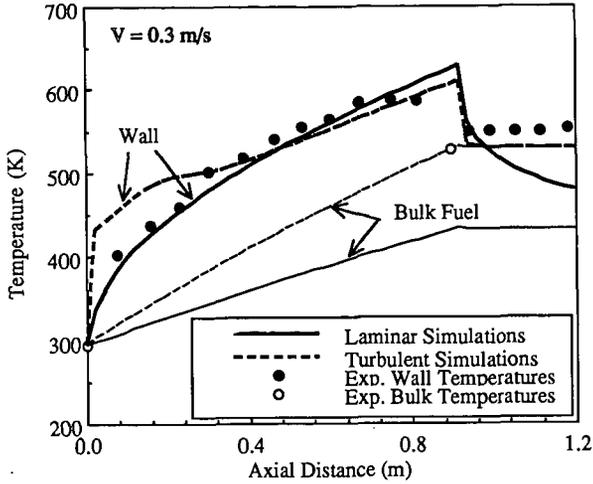


Figure 3. Comparison Between Predicted (Laminar and Turbulent Simulations) and Experimental Data for the Wall and Bulk Fuel Temperatures in the Heated Tube Experiment of Marteny (1989).

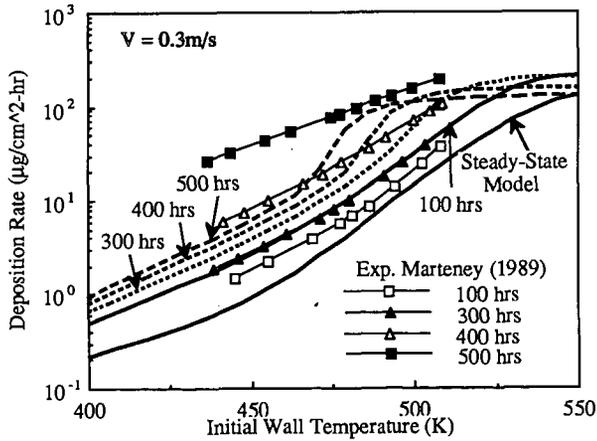


Figure 4. Predicted and Measured Deposition Rates for Long Duration Heated Tube Experiments of Marteny (1989).