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Incorporation of a Trade Study Tool for Fuels Development within *SRHEAT*™

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A Scramjet/Ramjet Heat Exchanger Analysis Tool (*SRHEAT*™) has been developed for rapid analyses of complex thermal cooling systems. Thermal management is critical to the development of dual-mode scramjets for hypersonic aerospace propulsion, which have high thermal loading with limited availability of heat sink sources. It is necessary that rapid trade studies of the thermal management system be accomplished to optimize the system for weight and cooling efficiency. To meet this need, *SPIRITECH* has developed a scramjet/ramjet heat exchanger design and optimization tool that performs a thermal analysis of the heat exchanger, assesses its structural strength, and optimizes the heat exchanger design to minimize the cooling flow requirement and the heat exchanger weight. *FuelDev*™ has been developed as an add-on to *SRHEAT*™ to provide a system level tool allowing fuels developers to experiment with fuel databases and to perform "what if" scenarios to determine the system level impacts of changes in fuel properties. *FuelDev*™ provides a tool to compare and contrast existing fuels for use in hypersonic vehicle thermal management systems. This tool provides the user with the ability to quantify the sensitivity of the thermal management system to changes in fuel properties afforded by new fuel technologies. The detailed heat exchanger design features included in the tools (i.e. geometry, material properties, fuel/coolant properties, etc.) make *SRHEAT*™ and *FuelDev*™ a valuable suite of tools in scramjet and hypersonic vehicle development, providing the low cost analytical capabilities that make possible the efficient development of aerospace components and fuels.

Nomenclature

A	=	pre-exponential Arrhenius factor
E_a	=	activation energy
k	=	first order reaction rate
R	=	gas constant
T	=	fuel temperature

I. Introduction

Managing the heat load to critical propulsion system components remains a significant challenge in the design and operation of a hypersonic vehicle. While a collection of thermal management strategies are available to the vehicle designer, weighing the effectiveness of those strategies and selecting the optimal approach early in the design process is time consuming and often uncertain due to design variable iterations. A Scramjet/Ramjet Heat Exchanger Analysis Tool (*SRHEAT*™) was created to address these challenges.[1] *SRHEAT*™ allows the vehicle designer to optimize the cooling system while considering the effects of flight point, engine geometry, material selection, fuel/coolant selection, cooling circuit routing, and heat exchanger geometry. The designer can assess the effectiveness of both passive (e.g. thermal barrier coatings) and active (fuel cooled liner panels) thermal management strategies through the use of metrics such as the required fuel flow rate, cooling system weight, and allowable structural stresses. In addition to interactive trade studies, *SRHEAT*™ can evaluate the performance of the

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cooling system over a range of design parameters, searching the design space for the optimal thermal management strategy.[2]

SRHEAT™ uses fundamental radiation, conduction, and convection modeling to accurately represent complex cooling systems and address scalability. Material property libraries are included to provide support for a wide variety of hydrocarbon-based and cryogenic fuels, and structural metals including high performance alloys.

SRHEAT™ is comprised of several modules:

- Engine Performance Module - calculates hot gas boundary conditions for heat exchanger panels and property distribution throughout the engine
- Flow Module - calculates fluid boundary conditions within heat exchanger panels, and fluid property distribution through a cooling circuit, including frictional losses and heating effects
- Thermal Module - calculates heat flux and temperature distribution within the heat exchanger panels
- Structural Module - calculates the stresses in the heat exchanger panels
- Optimizer Module - optimizes the coolant circuit order and the heat exchanger channel geometry
- Properties Module - provides a stored library of material and fuel properties for use within the thermal and flow modules

These modules employ the input from the user-friendly interface highlighted in **Error! Reference source not found.** to evaluate the performance of the user-defined cooling system. These features, along with the user-friendly interface, give the user the freedom to explore many hypothetical design changes rapidly, making *SRHEAT*™ a valuable tool in efficient hypersonic vehicle development.[3]

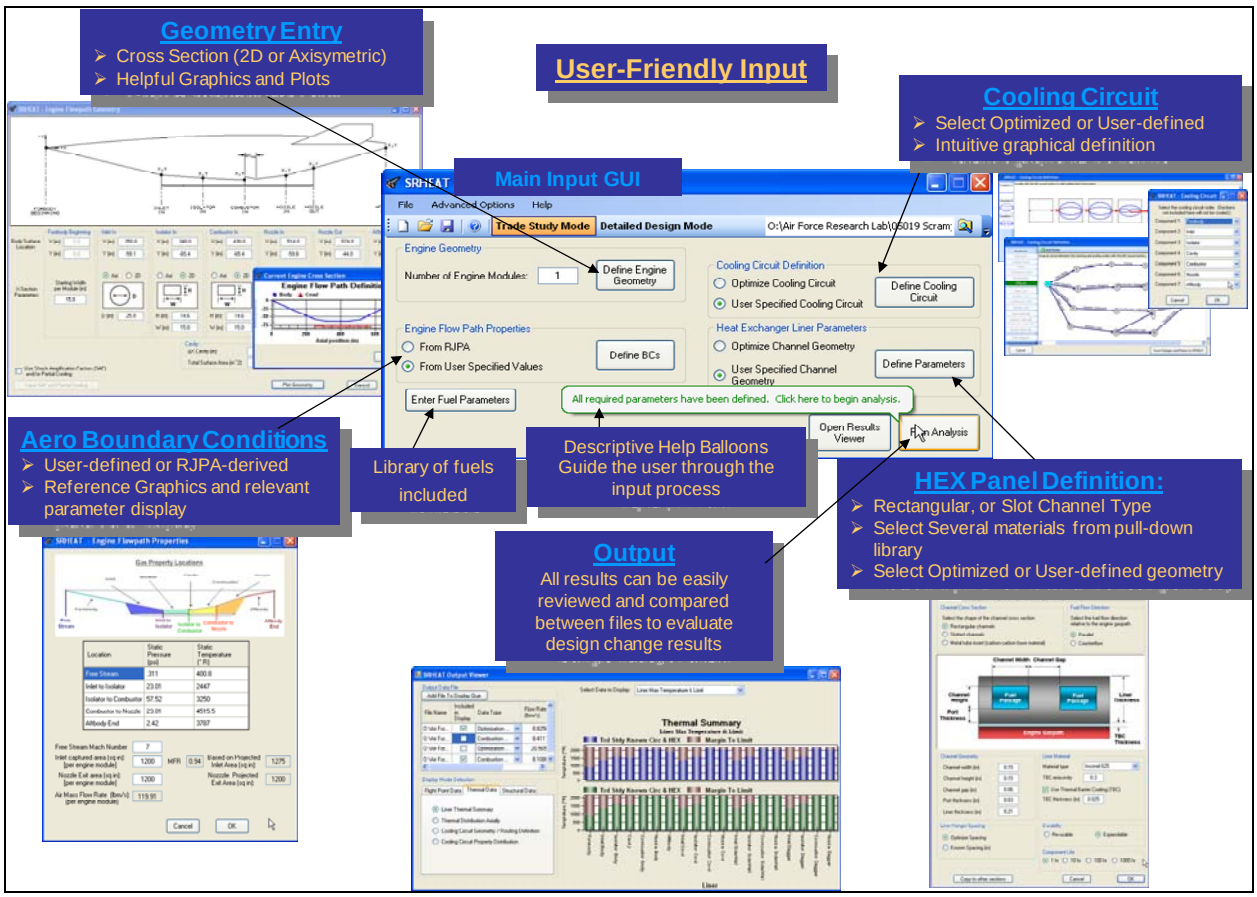

Figure 1. ***SRHEAT*™ Overview**

II. *FuelDev*™ Modeling

As discussed above, *SRHEAT*™ is capable of capturing the effects of a wide variety of design parameters on vehicle performance. It can be used for performing analyses such as optimization of cooling panel dimensions and trade studies to determine the effect of material selections on structural stability. However, the lack of chemical modeling in *SRHEAT*™ means that only modest heat loads on hydrocarbon fuels can be modeled. Higher heat loads cause *SRHEAT*™ to increase the fuel flow rate to prevent the fuel from entering its regime of thermal instability. While this approach was necessary in the initial development of *SRHEAT*™, *FuelDev*™ lifts this limitation and draws on the current experimental database of fuel decomposition to develop a more accurate physical model.

Since SRHEAT is a thermal management analysis tool, the largest impact of including a decomposition model will be the new capability of the code to consider the additional heat sink achieved through harnessing the endothermic decomposition reactions of hydrocarbon fuels. While the concept of utilizing fuel decomposition as a heat sink was initially proposed in the 1970s, only now do we have sufficient data to begin developing a semi-empirical physical model which can be incorporated into design tools to demonstrate the actual value of this advanced technology.[4]

While the experimental database of fuel decomposition research is still too sparse to develop any fundamental mechanism of JP fuel decomposition, there are sufficient data to utilize a global first-order Arrhenius model. For this, we rely on recent experiments which have determined decomposition rates and activation energies, GCMS analyses of product distributions after decomposition, and measurements of the heat absorbed during reaction. The model is described in detail in a later section. While simple, its power lies in its incorporation with *SRHEAT*™. Now we have a tool through which trade studies can be performed to determine the system level impacts of fuel decomposition, providing a practical assessment of this technology.

A. FuelDev Enhancements

FuelDev™ is an enhancement package which builds on the functionality of *SRHEAT*™, providing a valuable suite of tools that allows the fuels developer to quantify the system level impact of fuel decomposition in a fuel cooled sc/ramjet. The integration of *FuelDev*™ allows the user to take full advantage of the thermal and structural optimization algorithms present in *SRHEAT*™, with the novel ability to account for the influence of fuel properties as effected by both fuel selection and decomposition through the cooling system.

The objectives of the *FuelDev*™ package are to enhance the abilities of *SRHEAT*™ in the following ways:

1. **Develop and employ a model for fuel decomposition.**

   Several methods of modeling were explored. Due to the limitations of fuel decomposition research, an Arrhenius approach was adopted. This model is semi-empirical, requiring all necessary decomposition rates and endothermic heat sinks to be compiled from the literature.

2. **Account for the effect of decomposition on fuel properties.**

   Modeling decomposition required that *SRHEAT*'s existing property tables for JP-7, JP-8, JP-10, Jet-A, and RP-1 be greatly expanded to include fuel conversion as a state defining variable. Experimental product distributions from decomposition of each supported fuel are used to define surrogate decomposed fuels. SUPERTRAPP was used to generate the fuel property tables for the fuel surrogates, and must be updated with new surrogate component species if data permit. Tables for non-endothermic fuels supported by *SRHEAT*™ were updated to match the new table fidelity. To maintain a low runtime for each trade study, enthalpy tables were created for each fuel. All tables were created in a format that can be easily reproduced, allowing for the introduction of new fuels.

3. **Allow exploration of the system level impact of fuel properties.**

   To provide user access to the gamut of new features being included with *FuelDev*™, the fuel input GUI was updated. The new forms are depicted in Figure 2. In addition to maintaining basic fuel selection and boundary condition functionality, this form now allows the user to enable or disable decomposition routines. Independent options are given to control whether the effects of property changes due to decomposition and the endothermic heat sink are included. This allows comparisons to be made between the current decomposition model and previous enthalpy addition methods and lets the user gauge the importance of including decomposition models for any given fuel. The *Adjustable Fuel Parameters* subform adds the ability to apply weighting factors to fuel properties and Arrhenius parameters, enabling the user to weigh the system level effects of changes in fuel design. These adjustments can be saved as a new fuel, or reset to the nominal fuel properties. Through this form, the

user can use the weighting factors to explore conceptual fuels and determine what the properties of a high performing endothermic fuel should be.

4. Visualize effects of decomposition on the cooling system.

Current *SRHEAT*™ output forms were expanded to include the ability to plot fuel properties and state, including conversion, as a function of axial location in the combustion system. This allows the user to easily compare differences between several fuels and to pinpoint areas of rapid fuel decomposition. A fuel audit form is included to provide the properties of the fuel after leaving the cooling system in numerical form, which is valuable to injection modeling.

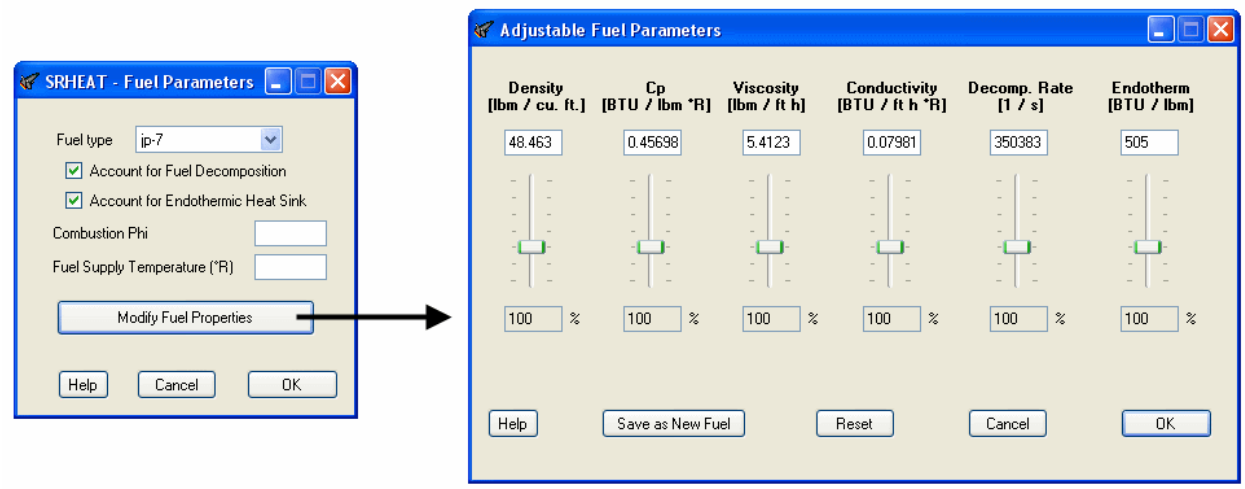

Figure 2. *FuelDev*™ Fuel Input Forms

B. FuelDev Modeling

1. Fuel Decomposition

When exposed to high temperatures, hydrocarbon fuels undergo a chemical change. Their constituent molecules begin to break down into lighter weight species, a reaction that is highly endothermic. While this thermal instability of hydrocarbon fuels is accompanied by system fouling through the buildup of coke on wetted surfaces, cracking can increase the available fuel heat sink by up to 50%.[5] Harnessing this additional heat sink in endothermic fuels is an enabling technology for sustained hydrocarbon fueled flight over Mach 4.[4]

Cracking changes the heat sink realizable by the fuel, not only due to the endothermicity of the reactions, but also due to changes in the thermophysical properties of the fuel as smaller species are formed. Both thermal and structural optimizations performed by *SRHEAT*™ are highly dependent upon the quantity of heat the fuel can absorb, so it is imperative to include modeling to capture both of these effects.

Early attempts at including the effect of endothermic fuel cracking in *SRHEAT*™ were achieved by simply increasing the fuel enthalpy as a function of temperature. This approach does not capture decomposition rates and assumes that fuel time-at-temperature in all *SRHEAT*™ simulations matches that of the experimental decomposition. Yet, even a simple model such as this significantly changes the fuel flow rate required to achieve sufficient cooling. Table 1 shows results for this analysis for a Mach 7 scramjet. Using this enthalpy model to include the contribution of endothermic reactions to the heat sink of the fuel causes a 17% reduction in the fuel flow rate required for cooling, with corresponding gains in the weight of the cooling system.

Table 1. Minimized Fuel Flow Rates for a Mach 7 Scramjet Including a Simple Enthalpy Addition Model for Fuel Decomposition.

Fuel	*Endothermic*	*Mach No.*	*Fuel Inlet Temp [ºR]*	*Fuel Outlet Temp [ºR]*	*Fuel Flow Rate [lbm/s]*	*Cooling System Weight [lbm]*
JP-7	No	7	520	1652	25.9	1305
JP-7	Yes	7	520	1635	21.4	1222

Developing a complete model of fuel decomposition is no simple task. Ideally, a complete decomposition mechanism would be used with a kinetics solver to determine the actual composition of the fuel after any history of thermal stress. This approach is not yet possible because decomposition is not fully understood. The composition of conventional jet fuels is too complex for complete pyrolytic mechanisms to be devised, although attempts have been made for the single JP-10 molecule.[6] Since *FuelDev*™ includes five JP grade fuels, a simpler approach applicable to all is required. Furthermore, solving a complete kinetic mechanism within *SRHEAT*™ would increase the runtime well beyond what is acceptable for a trade study tool.

It may be possible in the near future to develop and solve lumped mechanisms. In this approach, all product and intermediate species are lumped together into classes with similar structures, weights, and reactive pathways. This reduces the decomposition mechanism to a set solvable by current computational power in a reasonable time. However, it requires development of the reaction rates between the defined lumps, which is beyond the scope of this work.[7]

The state of the art of fuel decomposition research relies on an Arrhenius model for decomposition. In this approach, fuel decomposition rates are determined experimentally at several temperatures. First-order kinetics are assumed, and the data are fit to the well-known Arrhenius equation, Equation (1):

$$k = A \exp(-Ea/RT) \qquad \textbf{(1)}$$

where k is the decomposition rate, R is the gas constant, T is the fuel temperature, A is the pre-exponential factor, and Ea is the activation energy. By adopting Arrhenius parameters from literature (Table 2), the fuel decomposition rate is modeled as a function of temperature. Arrhenius parameters have been published for four of the fuels supported by *FuelDev*™, JP-8, Jet-A, RP-1, and JP-10. Direct measurements of JP-7 decomposition are lacking, but Arrhenius parameters for JP-7 have been inferred from the three species commonly used to comprise a surrogate for this fuel: n-decane, n-dodecane, and n-butylcyclohexane.[8] Knowing the decomposition rate and the total energy required to fully crack the fuel, *SRHEAT*™ can calculate the rate of heat absorption and modify the energy calculations within the flow model accordingly.

As the fuel is heated, these rates determine the conversion of any of the supported fuels into a selection of product species. Assuming that initial fuel decomposition is rapid when compared to interactions between the product species, then experimentally determined ratios of product species can be applied to calculate the composition of the fuel during and after thermal stress.[9] These compositions can be used to capture the effects of decomposition on the fuel properties.

JP fuels have been shown to fit first order kinetics well, so this approach is a good first pass at decomposition modeling.[9] However, several influences on decomposition rates are not taken into account. The adopted Arrhenius parameters are empirical values determined by thermally stressing aliquots of fuel in vessels presumed to be inert, usually Inconel. Decomposition rates are known to be affected by wall material. For example, fuel with a significant sulfur fraction (JP-8, Jet-A, RP-1) cooling copper liners would have a different decomposition rate due to catalytic effects. *SRHEAT*™ does allow the user to select liner materials, but their effect on fuel decomposition is currently not modeled.

Furthermore, the Arrhenius parameters are for thermal decomposition. Any catalytic effects, such as suspended catalysts or coatings or liquid phase additives that function to initiate decomposition reactions, are not directly modeled. Their net effect can be approximated, however, by adjusting the decomposition rate or endotherm in the *Adjustable Fuel Parameters* form.

Fuel decomposition goes hand in hand with fuel system fouling. The buildup of coke on wetted surfaces is a major limitation to real systems. The mechanisms of coke formation are being studied in the literature, and the dependencies of the rates of coke formation on flow conditions are currently being evaluated.[10,11] In *FuelDev*™, coking is currently handled by setting an upper limit on the fuel bulk temperature. This is the temperature at which coking has been experimentally shown to occur at a catastrophic rate. If fuel temperatures ever rise above this limit, *SRHEAT*™ increases the fuel flow rate. In the future, this could be replaced with an empirical coking model to

predict system lifetime and to model the effects of the thermal resistance of the coke layer within the fuel channels. Coking rates are as yet unpredictable, since they depend on flow parameters, wall materials, surface roughness, and temperature gradients and the experimental database does not adequately cover the possible combinations of these parameters.

Table 2. Arrhenius Parameters Utilized in Fuel Decomposition Modeling.

Fuel	A [1/s]	Ea [kJ/mol]	Source
JP-8	8.41×10^{7}	158	12
Jet-A	4.10×10^{12}	220	9
JP-10	2.40×10^{13}	256	13
RP-1	1.90×10^{15}	277	14
JP-7	5.31×10^{15}	270	15, 16, 17

2. Property Tables

As the composition of the fuel changes, the properties will change profoundly. Thermophysical properties of decomposed hydrocarbon fuels have not been experimentally measured; therefore, an approach to generate the necessary property tables is developed. Two tools have been created by NIST which allow the properties of hydrocarbon blends to be calculated: SUPERTRAPP and REFPROP. Defining the composition of the fuel in terms of component species concentrations for varying degrees of conversion allows use of these tools to determine the properties of the fuel.

Experimentally determined decomposition product distributions have been pulled from the literature for each fuel. Unfortunately, REFPROP currently does not contain many of the species necessary for calculation of properties of JP fuel surrogate mixtures. REFPROP does not allow the user to input new fuel species, so it could not be used for this application. The SUPERTRAPP library does provide properties of the majority of the necessary species, with three additional species (cyclohexene, cyclopentene, and 1-methylcyclohexene) being defined using appropriate critical properties and collision parameters from the literature.[18,19]

Fuel product distributions cannot be used directly in the generation of property tables, as decomposition results in an unmanageable number of product species for every fuel of interest. Surrogate fuels with a reduced number of components must be developed in order to complete this model. The challenge is to choose a selection of species such that all structural classes of molecules and the properties of the bulk phase are captured.

In developing these surrogates, it was assumed that the species distributions comprising the fuel surrogate and the decomposed fuel are frozen. Rather than attempting to model the potential complex interactions between the decomposition products once they form, it is assumed that the adopted global Arrhenius rate equation suffices. This assumption is supported by experimental decomposition analyses in which the decomposed product suite is seen to be nearly identical regardless of the time the fuel spent undergoing decomposition.[9]

This assumption allows determination of the composition of the fuel at any stage of conversion by mass weighting the surrogate components. Species concentrations for neat and fully decomposed fuels are developed from extensive lists in the literature, whereas intermediate species concentrations are calculated based on mass conversion.

JP-10 species compositions in mass fractions are presented in Table 3. Neat fuel is assumed to be pure exotetrahydrodicyclopentadiene, with no endo isomer or adamantane present. The product distribution presented in the bottom section of this table is adopted from Nageswara Rao & Kunzru.[20] A species comprising ~7% of the product stream was not included in our surrogate as it was unidentified by the authors. The concentration of three species (2-butene, isobutylene, and 1,3-butadiene) was reported as a single group, so we assumed equivalent mole fractions of these species in the surrogate. Cyclopentene was added to the SUPERTRAPP library to accommodate this surrogate. It is important to note that one of the products, cyclopentadiene, is known to decompose at high temperatures. This effect is not currently modeled, but the decomposition rate of this species is expected to be negligible at temperatures below the coking limit of JP-10.

RP-1 species compositions in mass fractions are presented in Table 4. The neat fuel surrogate, comprised of the first 10 species, was adopted from Edwards & Maurice.[21] The product surrogate was developed from Andersen & Bruno, with n-hexylcyclopentane (2.7% of the products by volume) lumped into n-heptylcyclopentane, and pentamethylbenzene (1.3% by volume) lumped with hexamethyl-benzene.[14] Specific species were not reported for

C11 and C12 bicycloparaffins, so these were modeled as 2-methyldecalin. Dimethylnaphthalene is assumed to be (2,6-) due to its presence in the SUPERTRAPP library. 1,3-dimethylcyclopentane is assumed to be (cis-). These species account for the entire gas phase except for methane, which was unresolvable by their technique.

Jet-A species compositions in mass fractions are presented in Table 5. Species concentrations were adopted from Widegren & Bruno.[9] No product species were lumped, as only the 10 most abundant out of 30 identified species were reported. Isodecane is assumed to be 3,3,5-trimethylheptane due to availability in the SUPERTRAPP library. The neat fuel surrogate was built from GCMS presented by the authors. Mass spectra were gathered from NIST and used to convert the authors' TIC results to approximate mass fractions.

JP-8 species compositions in mass fractions are presented in Table 6. The neat fuel surrogate was adopted from Huang, Spadaccini & Sobel.[5] This is the most complete surrogate, but it lacks isoalkanes. Tert-butylbenzene (5% by weight) was lumped with isobutylbenzene. Decomposition products of JP-8 have not been studied, so Jet-A decomposition products were duplicated here.

JP-7 species compositions in mass fractions are presented in Table 7. Decomposition product distributions have not been measured for JP-7, but by adopting a neat fuel surrogate from Mawid, we have been able to piece together a surrogate for the decomposed fuel.[8] This surrogate is comprised of three species, and thermal decomposition products for each of these species have been independently determined.[15,16] Summing product species when possible and lumping others allowed an approximate picture of JP-7 decomposition to be developed. For this, cyclohexene and 1-methylcyclohexene were added to SUPERTRAPP using data from the literature. At full conversion, a small concentration of fuel species remains due to dodecane decomposing into undecane and decane, and butylcyclohexane decomposing into vinylcyclohexane and allylcyclohexane. Since it was assumed that products of initial decomposition do not further decompose, these species are present in both the neat and decomposed surrogates. While a large number of species needed to be lumped with other species present in SUPERTRAPP, their total contribution to the decomposed fuel was small. Using this approach, 84.7% of the species by mass were directly accounted for.

With the surrogates defined, SUPERTRAPP was used to generate property tables. Fuel species concentrations were calculated from 0 to 100% conversion in 10% increments. The temperature domain covers 300ºR < T < 1800ºR in 25º increments. Pressure runs from 300 to 1000 psia in 100 psi increments, then to 4500 psia in 500 psi increments. The net result of this grid is a maximum error in property interpolation of 5% at the supercritical point, with error below 0.5% for over 95% of the table domain.

Table 3. JP-10 Surrogate

exotetrahydrodicyclopentadiene	1.0000
cyclopentadiene	0.1542
propylene	0.2076
ethylene	0.2675
methane	0.1745
toluene	0.0292
ethane	0.0745
cyclopentene	0.0329
benzene	0.0258
trans-2-butene	0.0066
propane	0.0076
1-butene	0.0060
2-methylpropene	0.0067
1,3-butadiene	0.0069

Table 4. RP-1 Surrogate

n-undecane	0.0454
n-dodecane	0.0537
n-tridecane	0.1571
n-tetradecane	0.1191
heptylcydopentane	0.0614
octylcyclopentane	0.1008
nonylcyclopentane	0.0629
2-methyldecalin	0.3121
mexamethylbenzene	0.0345
2,6-dimethylnaphthalene	0.053
propane	0.6117
isopentane	0.1994
2-methylpentane	0.0523
n-hexane	0.0516
methylcydopentane	0.0233
benzene	0.0274
cis-13-dimethylcyclopentane	0.0082
n-heptane	0.0104
methylcydohexane	0.0082
toluene	0.0075

Table 5. Jet-A Surrogate

n-pentadecane	0.0336
n-tetradecane	0.0734
n-tridecane	0.0850
n-dodecane	0.0948
n-undecane	0.0643
n-nonane	0.0508
3,3,5-trimethylheptane	0.1330
isobutylcyclohexane	0.0387
1,2,4-trimethylbenzene	0.3644
1,2,3,4-tetrahydronaphthalene	0.0620
n-butane	0.1708
n-pentane	0.1393
propane	0.1367
isobutane	0.1130
isopentane	0.1064
ethane	0.0867
n-hexane	0.0841
2-methylpentane	0.0775
methylcydopentane	0.0434
3-methylpentane	0.0421

Table 6. JP-8 Surrogate

methylcyclohexane	0.0750
meta-xylene	0.0700
n-octane	0.1300
n-decane	0.1560
butylbenzene	0.0550
isobutylbenzene	0.1100
n-dodecane	0.1750
1-methylnaphthalene	0.0520
n-tetradecane	0.1120
n-hexadecane	0.0650
n-butane	0.1708
n-pentane	0.1393
propane	0.1367
isobutane	0.1130
isopentane	0.1065
ethane	0.0867
n-hexane	0.0841
2-methylpentane	0.0775
methylcyclopentane	0.0434
3-methylpentane	0.0420

Table 7. JP-7 Surrogate

n-decane	0.2173
n-dodecane	0.3258
n-butylcyclohexane	0.4569
n-decane	0.0107
n-dodecane	0.0001
n-butylcyclohexane	0.0179
1-methylcyclohexene	0.0996
ethane	0.0879
cyclohexane	0.0779
1-hexene	0.0722
methane	0.0590
ethylene	0.0579
propane	0.0594
1-pentene	0.0621
propylene	0.0604
1-heptene	0.0630
1-octene	0.0439
cyclohexene	0.0411
1-nonene	0.0335
methylcyclohexane	0.0307
1-decene	0.0308
n-pentane	0.0508
hydrogen	0.0411

C. FuelDev Validation

Comparison of the *FuelDev*™ model against physical data is difficult, as decomposition data are scarce, and most sources were used while adopting Arrhenius parameters and creating surrogates. Assessing decomposition predictions from the model against the data used to generate the decomposition rates would prove little use. Fortunately, two sources exist which permit comparisons for the adopted surrogates and the decomposition model.

As a sanity check, *FuelDev* JP-8 and Jet-A surrogates can be compared to both other surrogates and actual fuel samples by comparing their density as a function of temperature, ignoring decomposition. Figure 3 is reproduced from Edwards[22] with densities of the *FuelDev* Jet-A and JP-8 surrogates overlaid. The JP-8 surrogate was adopted from Huang, Spadaccini & Sobel.[5] When used in SUPERTRAPP, this surrogate results in densities lower than others, but within ~4% of the average. *FuelDev*'s Jet-A surrogate, which was developed by lumping together the 46 species reported as GCMS counts by Widegren[9] into 10 species, shows good agreement with other surrogates and experiment.

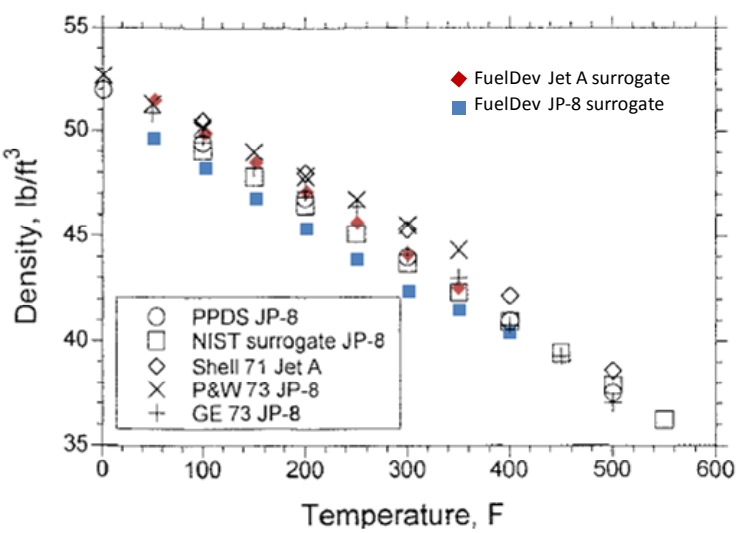

Figure 3. Surrogate Density Comparison vs. Other Sources. [Edwards *et al.*, 2001]

The accuracy of the decomposition models incorporated into *FuelDev*™ was demonstrated by using the code to reproduce the conditions of a thermal cracking experiment. Figure 4 is a plot from Edwards[23] showing the extent of thermal cracking of JP-7 after flowing through a heated stainless steel tube with a given fuel exit temperature. The flow conditions (900 psia, 30 mL/min, 0.9s residence time, 600°F fuel inlet temperature) were reproduced in *FuelDev*™ and the heat flux into the fuel was adjusted. This gives both a conversion percent and the fuel exit temperature. The conversion was then weighted by the proportion of the decomposed JP-7 surrogate that would be gas phase at the fuel sample conditions, and the results are overlaid on Figure 4. At the highest fuel exit temperatures, *FuelDev*'s decomposition model matches experiment. However, the model does predict decomposition to start at a lower temperature than was seen in this experiment. This is not surprising, as JP-7 Arrhenius parameters were estimated from the three components of the surrogate. This surrogate includes n-decane which begins to decompose at 1020°F.[15]

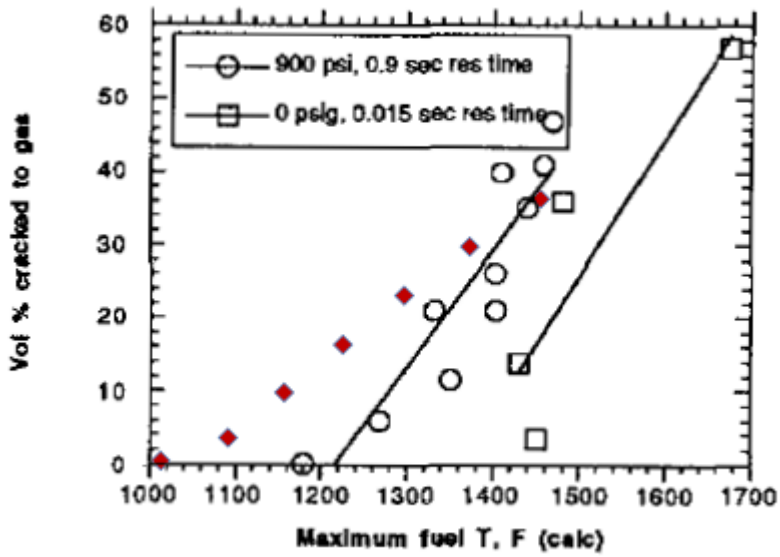

Figure 4. Validation of JP-7 Thermal Cracking. [Edwards and Anderson, 1993]

III. *FuelDev*™ Demonstration

A. Decomposition Modeling

Integration of the *FuelDev*™ package has enhanced the capabilities of *SRHEAT*™ to account for the effects of fuel decomposition. Both property changes and increased heat sink due to the endothermic nature of the cracking reactions are included, bringing the thermal analyses performed by *SRHEAT*™ closer to reality. To highlight these new features and to gauge the impact of fuel decomposition modeling on high Mach vehicle design, we present several demonstration cases.

Our first case study will use a representative Mach 7 scramjet design to highlight the new features *FuelDev*™ brings to the *SRHEAT*™ output forms. The fuel path through the cooling panels proceeds in a simple fore-to-aft fashion for maximal clarity in the output. JP-7 is the selected fuel. *SRHEAT*™ performs the thermal analysis to determine the fuel flow rate required to provide sufficient cooling to the propulsion system. This analysis is run twice: first without decomposition modeling and second with decomposition modeling enabled.

Figure 5 shows a screenshot of the *SRHEAT Output Viewer* with results from these two analyses displayed. The upper left of the form contains a short summary of the analyses. From this summary, we see that the case without decomposition modeling requires a fuel flow rate of 0.3182 lbm/s to provide sufficient cooling to the propulsion system, whereas the case with decomposition modeling requires 0.1739 lbm/s. This 45% reduction in cooling flow highlights the major potential of endothermic fuel technology.

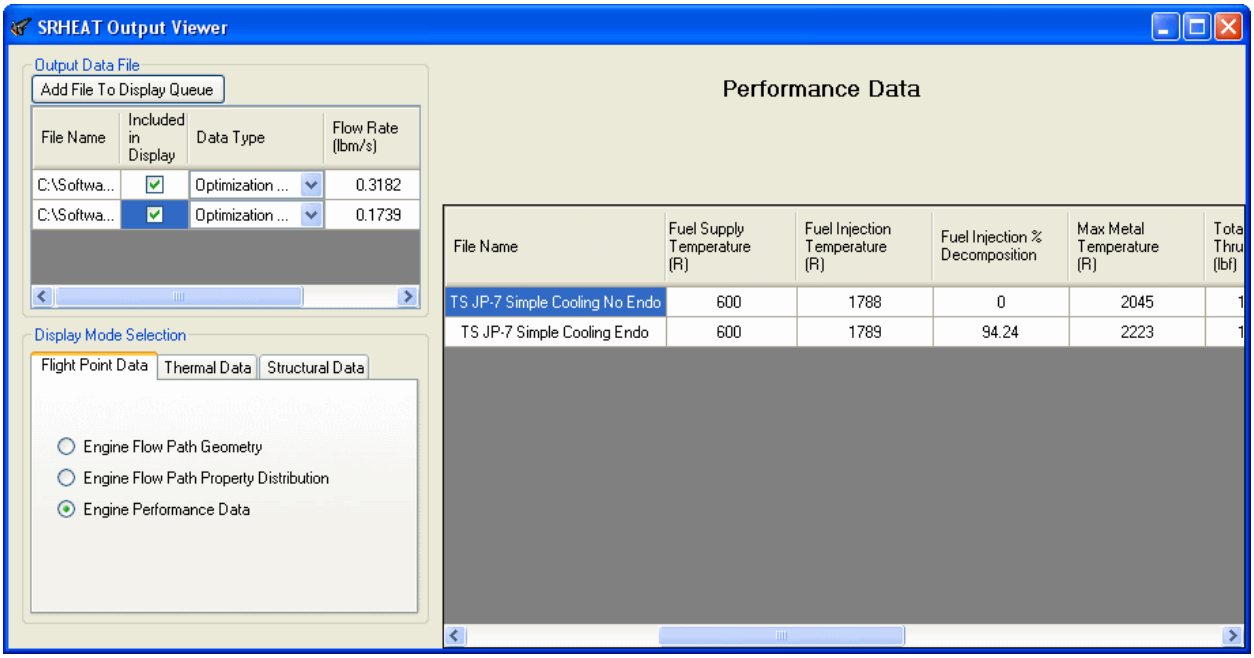

Figure 5. Output Viewer – Engine Performance Data

The *SRHEAT Output Viewer* gives the user the ability to quickly access and compare performance analysis results and the boundary conditions defined for each case loaded into the viewer. The lower left of the form provides access to a collection of summary forms grouped by discipline. In Figure 5, *Engine Performance Data* is selected, which gives the user access to propulsion system parameters such as air flow rate, thrust, and I_{sp}. *FuelDev*™ expands on this summary by including net fuel changes such as the fuel temperature and conversion upon exiting the cooling system. Here we see the reason for the large decrease in fuel flow rate required for cooling: the analysis with decomposition modeling enabled predicts the fuel conversion to be over 94% when the fuel leaves the cooling panels. In a real system, this level of decomposition would be accompanied by serious system fouling. The system designer may wish to pinpoint the areas of highest decomposition rates and address this issue by using a liner material more resistant to coking or by adding a fouling resistant coating.

FuelDev™ has added a new display mode which can handle exactly this sort of analysis. As shown in Figure 6, the *Fuel Property Distribution* display mode allows the user to examine the state of the fuel through each liner in detail. Up to four parameters may be plotted at a time from the set of conversion, temperature, pressure, density, specific heat, viscosity, and thermal conductivity. The selected properties are plotted for a single liner, selected by the user at the top of this form. By stepping through the liners, one is able to see that decomposition is not a significant effect in the cooling system until the fuel reaches the combustor liner, as shown in Figure 6. This can be confirmed by plotting the fuel temperature in each upstream liner. In each, the fuel temperature remains below 1250°R, meaning the temperature regime of decomposition has not yet been reached.

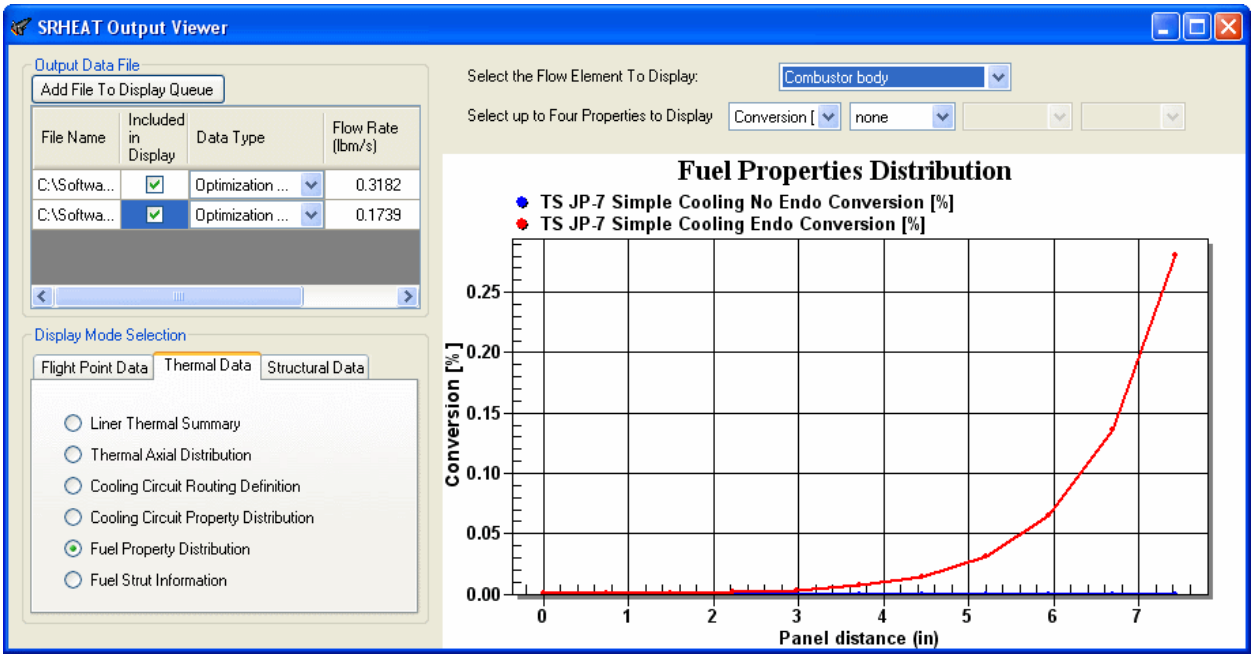

Figure 6. Output Viewer – Fuel Property Distribution, Combustor Liner

Continuing through the liners, one can also identify the nozzle liner as the largest contributor to fuel decomposition. As shown in Figure 7, the fuel conversion increases from 6% to 82% over the course of this liner. This result can be confirmed by visiting the *Liner Thermal Summary* mode, which shows that the nozzle liners are under the largest thermal load and have the highest wall temperature of any liners in this sample case. By using the *Fuel Property Distribution* display mode included with *FuelDev*™, the user is able to examine the state of the fuel as it flows through the cooling system and rapidly identify potential design issues.

A major feature of *SRHEAT*™ is its ability to optimize certain fundamental parameters of the cooling system. For example, the cooling circuit, or order in which the fuel passes through the liner panels, has a large impact on temperature gradients between the fuel and the liners. Since these gradients drive the heat transfer to the fuel, a non-obvious circuit order may have a much more effective cooling capacity than a simpler design. The optimal circuit order becomes even less clear when fuel decomposition is considered. *FuelDev*™ is not just an add-on package; it is a new chemical model allowing the impact of fuel decomposition to be included during initial design iterations.

Figure 8 shows the *Cooling Circuit Routing Definition* display mode, which allows the user to view the circuit order for each case. The top right of the image shows the fore-to-aft cooling circuit which we had specified in the previous demonstration. The lower right of the image shows the cooling circuit devised by *SRHEAT*™ when allowed to optimize the circuit order with decomposition reactions enabled. Here we see that, in general, the liners with the highest heat loads have moved to the front of the circuit, though the entire circuit is not in order of decreasing heat loads. By using the *Fuel Property Distribution* display mode, we can determine that decomposition becomes significant within the nozzle liner panels and remains so throughout the entire cooling circuit. The net result of utilizing the endothermic heat sink throughout the cooling system is a reduction in the fuel flow rate required for cooling to 0.1684 lbm/s. For this particular example, whether this savings over the fore-to-aft cooling flow rate of 0.1739 lbm/s is worth the added system complexity and plumbing weight is debatable. However, the power of this tool is its ability to rapidly consider these effects early on in the design process.

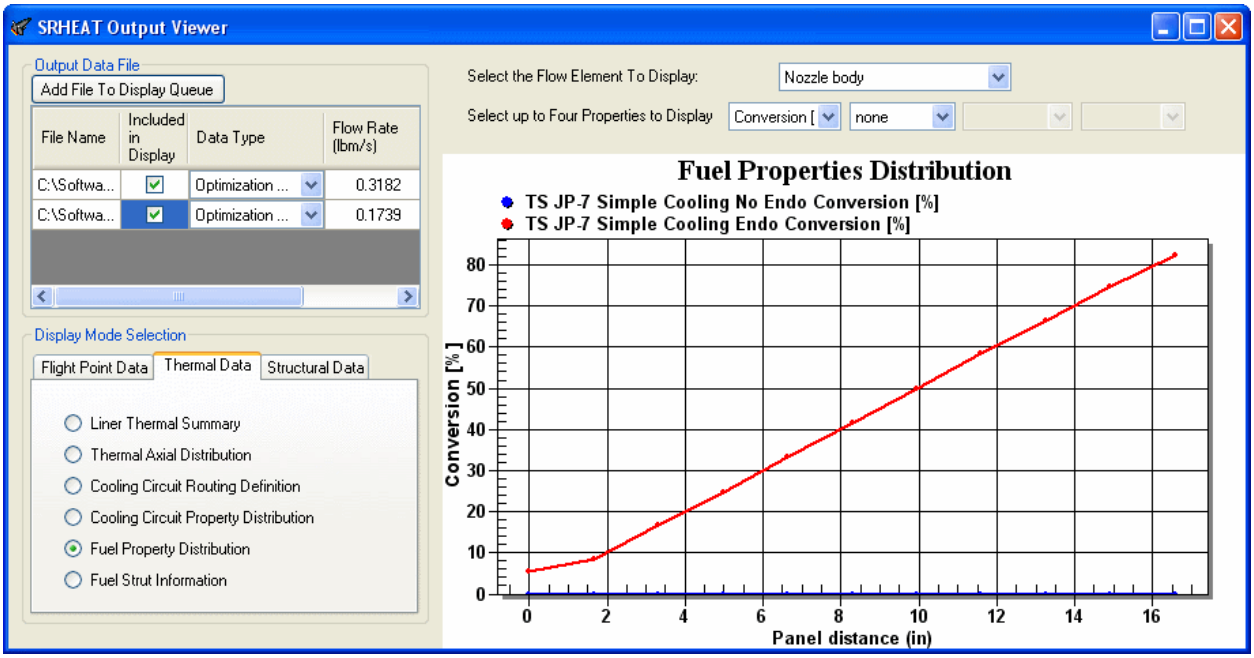

Figure 7. Output Viewer – Fuel Property Distribution, Nozzle Liner

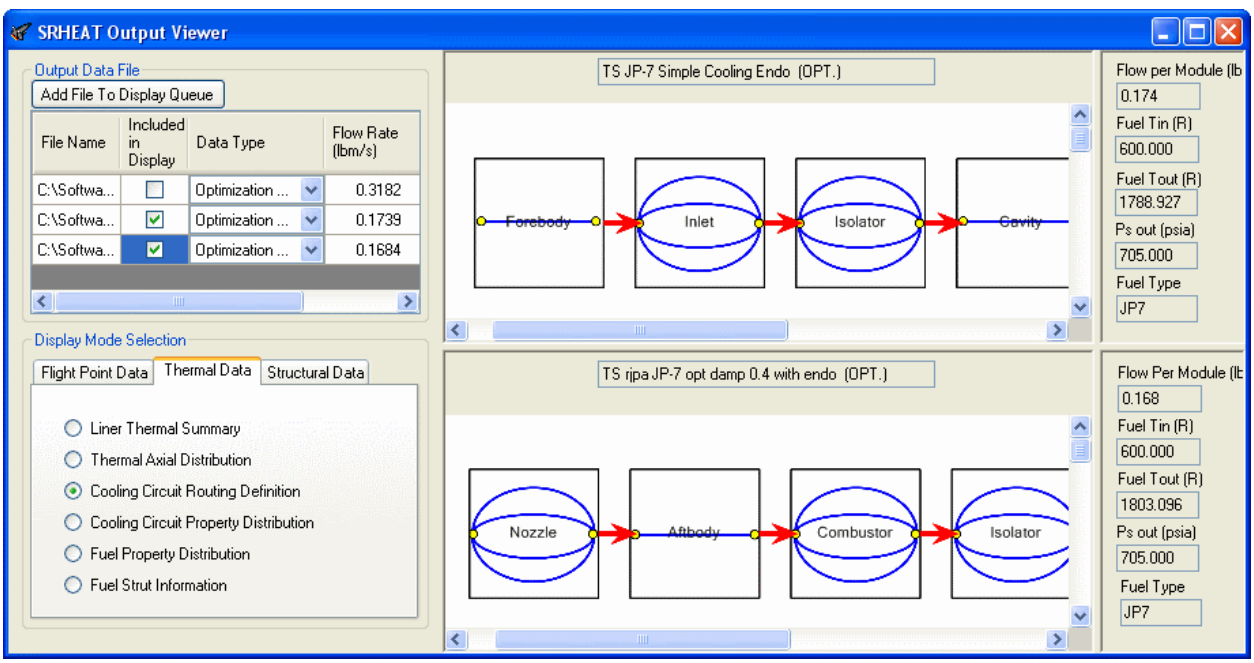

Figure 8. Output Viewer – Cooling Circuit Routing Definition

B. Fuel Property Exploration

In addition to decomposition models, *FuelDev*™ includes a feature which allows the user to artificially adjust fuel properties to examine the system level effects of small adjustments to the fuel. Figure 9 shows plots of fuel density versus axial combustor location for three tests using JP-7. In two of these tests, the density of the fuel has been weighted by factors of 0.9 and 1.1. All other conditions being equal, increasing the fuel density is expected to increase its cooling capacity. This effect manifests itself as a decrease in the required fuel flow rate to provide cooling, as shown in Figure 9. Here, the direct effect of modifying the density is confirmed using the *Fuel Property Distribution* display mode. The fuel flow rate required for cooling for our nominal case is 0.1725 lbm/s. A 10%

decrease in the fuel density causes the flow rate to increase to 0.1747. A 10% increase in the fuel density causes the flow rate to decrease to 0.1724. While this qualitative trend was expected, *FuelDev*™ allows the user to quantify the effects of hypothetical scenarios such as this. By continuing this logic, the fuels developer can use *FuelDev*™ to focus in on the properties of an optimum endothermic fuel. Changes to fuel density, viscosity, conductivity, specific heat, rate of decomposition, and enthalpy of decomposition are currently supported.

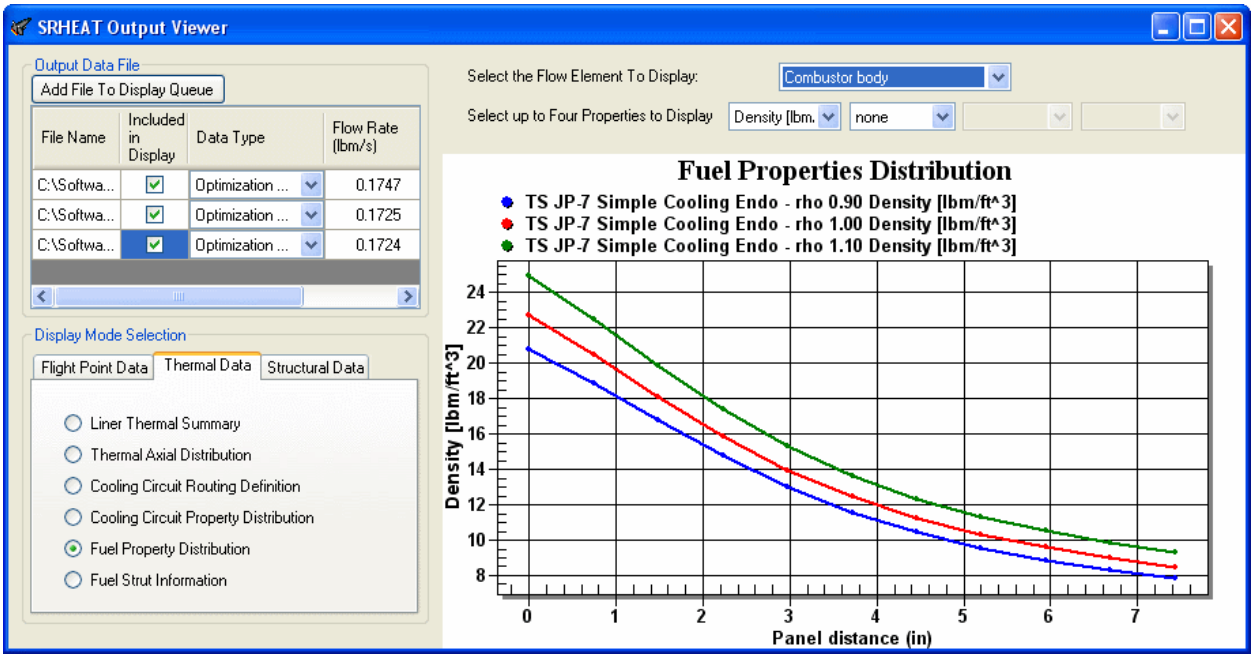

Figure 9. Effect of Increases in Fuel Density on Required Fuel Flow Rate.

IV. Conclusions

A Scramjet/Ramjet Heat Exchanger Analysis Tool (*SRHEAT*™) has been developed for rapid structural and thermal analyses of complex thermal cooling systems. The analytical model provides a multidisciplinary system level thermal analysis that balances the heat load from the gas path, through the liners, and into the fuel. The heated fuel is injected into the gas path for combustion to complete the closed-loop thermal system. Detailed thermal and structural analyses are performed to accurately size the system for the desired mission and life requirements.

This user-friendly design tool was developed with ease-of-use as a primary focus. Simple, drop-down menus for selecting the coolant fuel, including its associated endothermic properties, are used so that various fuels may be easily evaluated. In addition, drop-down menus are also included for selecting various high temperature material properties. The user-friendly interface simplifies the use of *SRHEAT*™ for performing large trade studies. Using numerical optimization techniques, the code can define the optimum configuration to minimize weight and required cooling fuel flow for the user-defined boundary conditions, or the user may select to run a specific configuration at off-design conditions.

Integration of the *FuelDev*™ package has enhanced the capabilities of *SRHEAT*™ to account for the effects of fuel decomposition. Both property changes and increased heat sink due to the endothermic nature of the cracking reactions are included, bringing the thermal analyses performed by *SRHEAT*™ closer to reality. *FuelDev*™ builds on the functionality of *SRHEAT*™, providing a valuable suite of tools that allows the developer to quantify the system level impact of decomposition in a fuel cooled scramjet. The integration of *FuelDev*™ allows the user to take full advantage of the thermal and structural optimization algorithms present in *SRHEAT*™, with the novel ability to account for the influence of fuel properties as effected by both fuel selection and decomposition through the cooling system.

The *FuelDev*™ package provides the developer with the following features:

1. Quick and easy comparison of different fuels.
2. Quantification of the system level impact of variations in properties for a particular fuel, providing insight toward optimal fuel properties for vehicle cooling applications.
3. A library of conventional fuel properties.
4. The ability to import a user-defined fuel property table, allowing simulation of any imaginable fuel.
5. Global fuel decomposition models including the effect of fuel heat sink capacity.
6. Assessment of the changes in fuel composition and properties due to thermal stress.
7. The option to disable decomposition models, allowing the user to determine whether decomposition models are necessary for an accurate thermal solution.
8. User-friendly output forms, showing the impact of the fuel definition on key metrics.
9. User-friendly interface.

V. Future Plans

While *FuelDev*™ provides marked improvements in scramjet thermal analysis by including fuel decomposition modeling, future work could further enhance this tool for both the fuels developer and system designer. Several physical ramifications of decomposition could be included in future revisions of *FuelDev*™. Currently, *FuelDev*™ is capable of modeling the change in properties and composition of the fuel due to thermal stress. But as a fuel cracks into lighter species, its combustion time will decrease, resulting in a change in the gas path heat loads and a reduction in the optimum combustion chamber length. This impact is currently ignored in *SRHEAT*™, as the gas path is calculated in RJPA using the neat fuel. It would be desirable and possible to remove the current dependency on RJPA and develop an improved gas path model that can account for effects of fuel decomposition.

The decomposition model included in *FuelDev*™ currently handles the rate and thermal impact of fuel cracking, but does not attempt to model coking. Currently, an upper temperature limit is defined for each fuel, at which fuel coking is assumed to proceed at a catastrophic rate. While this effect is seen in experiment, the reality of the situation is more complex. The rate of coke build-up has been seen to be an exponential function of fuel conversion, making it a significant effect at temperatures well below the current limit.[23] Data permitting, future work could include a coking model to account for the slow build up of a coke layer at lower temperatures. It would be necessary to draw coking rates from the literature for each fuel, and for each wall material when possible. It would be possible to include the effects of protective coatings on wetted surfaces, and to include the thermal resistance of the coke layer in thermal analyses. With the integration of a coking model, *SRHEAT*™ could estimate system lifetime, if limited by fuel system fouling effects, such as plugging of the fuel channels, or insufficient liner cooling due to increased thermal resistance from coke build up.

In a related effect, much of fuel decomposition research currently focuses on the use of catalysts to optimizing fuel cracking rates. The state of the art is to use inexpensive zeolite catalysts coating the wetted surface of the fuel channels. The global effect of this is to lower the temperature at which fuel cracking becomes significant, which can be modeled in the current version of *FuelDev*™ by weighting the fuel decomposition rate. However, the catalysts of interest are silica-alumina based, meaning they have very low conductivities. In similar fashion to modeling a layer of coke on the wetted surface, the thermal impact of these catalysts could be modeled in future versions.

Minor improvements could be made to the current code as well. Plotting routines for *FuelDev*™ were adopted from the *SRHEAT*™ style, which are great for a systems analyst, but a fuels developer may wish to see this information from the perspective of the fuel. These plots could be revamped to show the effects of decomposition as a function of fuel residence time in the cooling system rather than as vehicle axial location. Furthermore, changes to the fuel can be included for all geometries overlaid at once rather than requiring individual plots. This would simplify interpretation of systems where the optimized fuel path does not proceed in a continuous manner along the vehicle axis.

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