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INFLUENCE OF TEST CONFIGURATION ON THE COMBUSTION CHARACTERISTICS OF POLYMERS AS IGNITION SOURCES

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ABSTRACT

The experimental evaluation of polymers as ignition sources for metals has been accomplished at the NASA White Sands Test Facility (WSTF) using a standard promoted combustion test. These tests involve the transient burning of materials in high-pressure oxygen environments. They have provided data from which design decisions can be made; data include video recordings of ignition and non-ignition for specific combinations of metals and polymers. Other tests provide the measured compositions of combustion products for polymers at select burn times and an empirical basis for estimating burn rates. With the current test configuration, the detailed analysis of test results requires modeling a three-dimensional, transient convection process involving fluid motion, thermal conduction and convection, the diffusion of chemical species, and the erosion of the sample surface. At the high pressure extremes, it even requires the analysis of turbulent, transient convection where the physics of the problem are not well known and the computation requirements are not practical at this time.

An alternative test configuration that can be analyzed with a relatively-simple convection model was developed during the summer period. The principal change constitutes replacing a large-diameter polymer disk at the end of the metal test rod with coaxial polymer cylinders that have a diameter nearer to that of the metal rod. The experimental objective is to assess the importance of test geometries on the promotion of metal ignition by testing with different lengths of the polymer and, with an extended effort, to analyze the surface combustion in the redesigned promoted combustion tests through analytical modeling of the process. The analysis shall use the results of cone-calorimeter tests of the polymer material to model primary chemical reactions and, with proper design of the promoted combustion test, modeling of the convection process could be conveniently limited to a quasi-steady boundary layer analysis where the economical solution of parabolic equations is involved.

The products for the summer period are: (1) a conceptual-level redesign of the test apparatus, and (2) the development and use of an approximate integral boundary layer analysis to demonstrate the influence of geometry changes prior to testing. A computer code STAN5, an accurate numerical boundary layer model whose earlier versions were developed for the NASA Lewis Research Center by the Fellow, also was installed and validated on the WSTF and New Mexico State University computer systems as a starting point in the development a more detailed fluid mechanics and combustion model.

INTRODUCTION

The standard promoted combustion tests performed at the White Sands Test Facility (WSTF) have been used by NASA, DOD and industry to select materials for oxygen systems where polymer materials are used for seals, seats, etc. The burning of metals in the presence of various burning polymers can be ranked with the data obtained. However, there is not a clear understanding of the importance of the test configuration on the test results or the possible influence of the configuration in the oxygen system of primary interest.

A redesign of the test configuration to facilitate a more convenient analysis of the test geometry and the combined fluid mechanics/combustion processes near the surface of the burning material was undertaken. The objectives for the summer period were to identify design changes and to demonstrate through a preliminary approximate boundary layer analysis that configuration dependent parameters must be considered.

An overview of the results of the investigation are described in this report, with specific details being available to the reader upon request. The design changes in the standard test are first described. This is followed by an outline of the approximate integral boundary layer analysis and the numerical results obtained for one representative polymer. Then, the more accurate numerical model STAN5 that was installed on the WSTF and New Mexico State University computer systems for future investigations is described. Conclusions and recommendations for future work are presented at the end of the report.

SYMBOLS

A	Surface area, m^2
b	Blowing parameter, defined in Eq. (8)
c_p	Specific heat at constant pressure, J/(kg K)
C_f	Friction factor, defined in Eq. (9)
F	Constants, defined in Eqs. (10)-(12)
g_c	Conversion constant in Newtons Second Law, kg m/s^2N
Gr_x	Local Grashof number, based on position x
i	Enthalpy, J/kg
i*	Stagnation enthalpy, J/kg
J	Conversion constant, work equivalent of energy
k	Thermal conductivity, $W/(m^2$ K)
m"	Mass flux, kg/m^2
m_j	Mass concentration of component j, kg per kg of mixture
P	Pressure, Pa
Q	Heat transfer rate, W
q"	Heat flux, W/m^2
r	Radial distance in cylindrical coordinates, m
T	Temperature, K
u	Velocity in x-direction, m/s
u'	Instantaneous value of fluctuating velocity component in x-direction, m/s
u_1	Characteristic velocity, m/s
v	Velocity in y-direction, m/s
v'	Instantaneous value of fluctuating velocity component in y-direction, m/s
X	Body force in x-direction, N

x	Distance along surface of body, m
y	Distance normal to surface of body, m
β	Volumetric coefficient of thermal expansion, K^{-1}
γ_j	Mass diffusion coefficient for substance j in a mixture, kg/(m s)
δ	Boundary layer thickness, m
ϵ	Emissivity of polymer surface
μ	Dynamic viscosity, (N s)/m^2
ν	Kinematic viscosity, m^2/s
ρ	Density, kg/m^3
σ	Stefan-Boltzmann constant, W/(m^2 K^4)
τ	Shear stress, Pa
ψ	Parameter, defined in Eq.

Subscripts:

e	Refers to entrained fluid at edge of the boundary layer
o	Refers to value at surface
R	Refers to radiation
∞	Refers to position outside boundary layer

DESCRIPTION OF TEST GEOMETRY AND THE PROPOSED CHANGES

Figure 1 is a sketch of the modified test chamber with the test samples shown. The changes made to the test chamber included:

- Addition of a top view port to analyze cumulative products of combustion for the purpose of calibrating and confirming the boundary layer analysis

- Addition of a quartz cylinder to collect and direct products of combustion to top view port.

The selection of instrumentation required for chemical analysis has not been made and the experimental evaluation of possible problems associated with gas collection in a quartz tube and the possible condensation of metals making the tube opaque have not been made. With these minimal changes, the test chamber should continue to provide for testing with gas pressures up to 69 MPa.

Another major change in the test involves replacing the flat disk polymer sample with a cylindrical polymer sample that is nearer the diameter of the metal rod sample. Figure 2 compares the current configuration with a proposed "carrot shape" configuration based on the integral boundary layer analysis performed. The proposed shape reflects a variable burning rate for the polymer that after a period of time will result in coaxial polymer and metal cylinder samples of equal diameter; at that particular instant in time, a quasi-steady boundary layer flow can be assumed and modeled. With this change, the effects test configuration can be evaluated by testing polymer samples of different length giving different thermal conditions at the polymer-metal interface.

Average burning rates were estimated for a polyethylene sample using measured burning rates for a disk sample recently tested by Shelly et al. (1993). The test samples

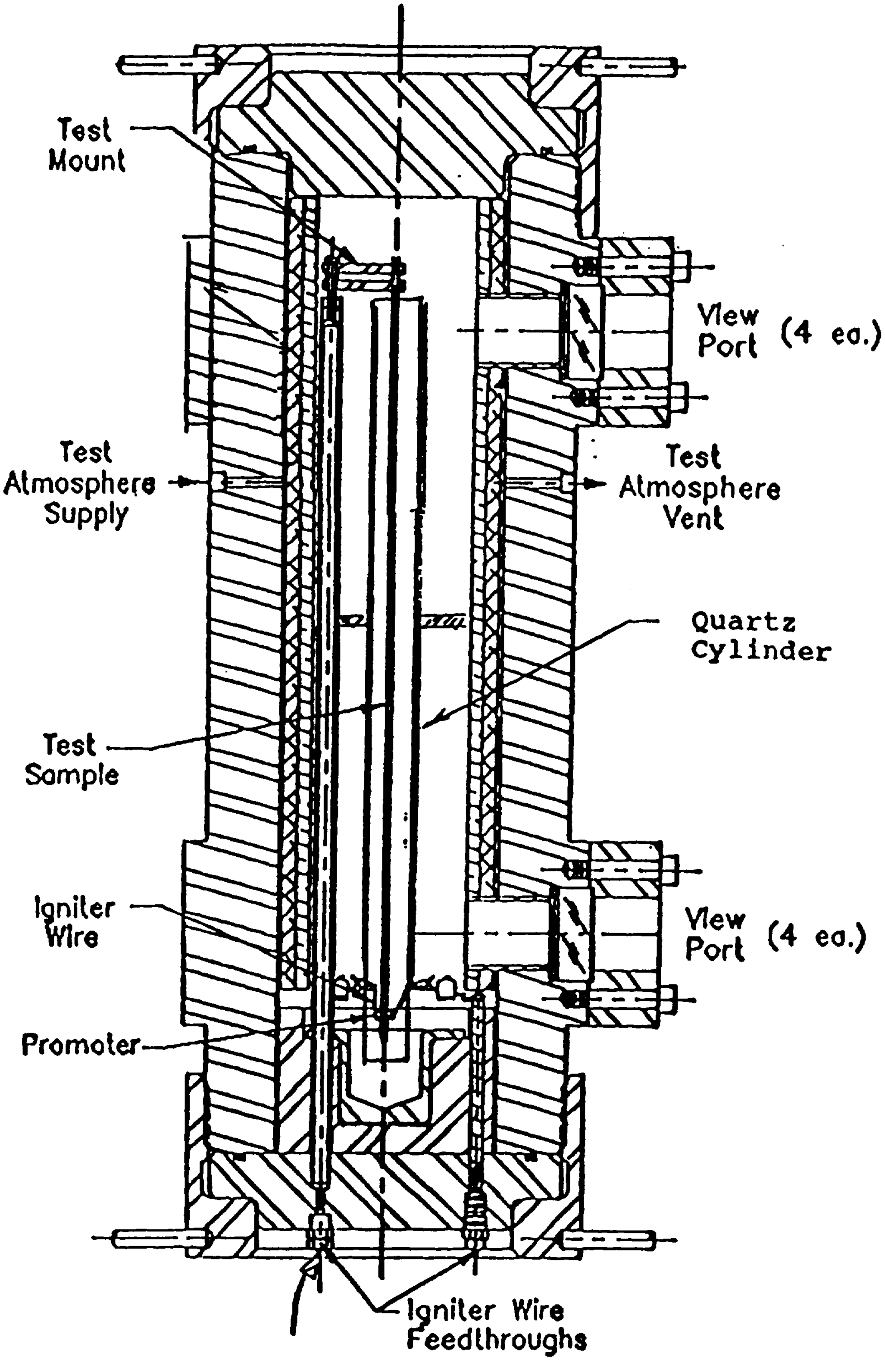
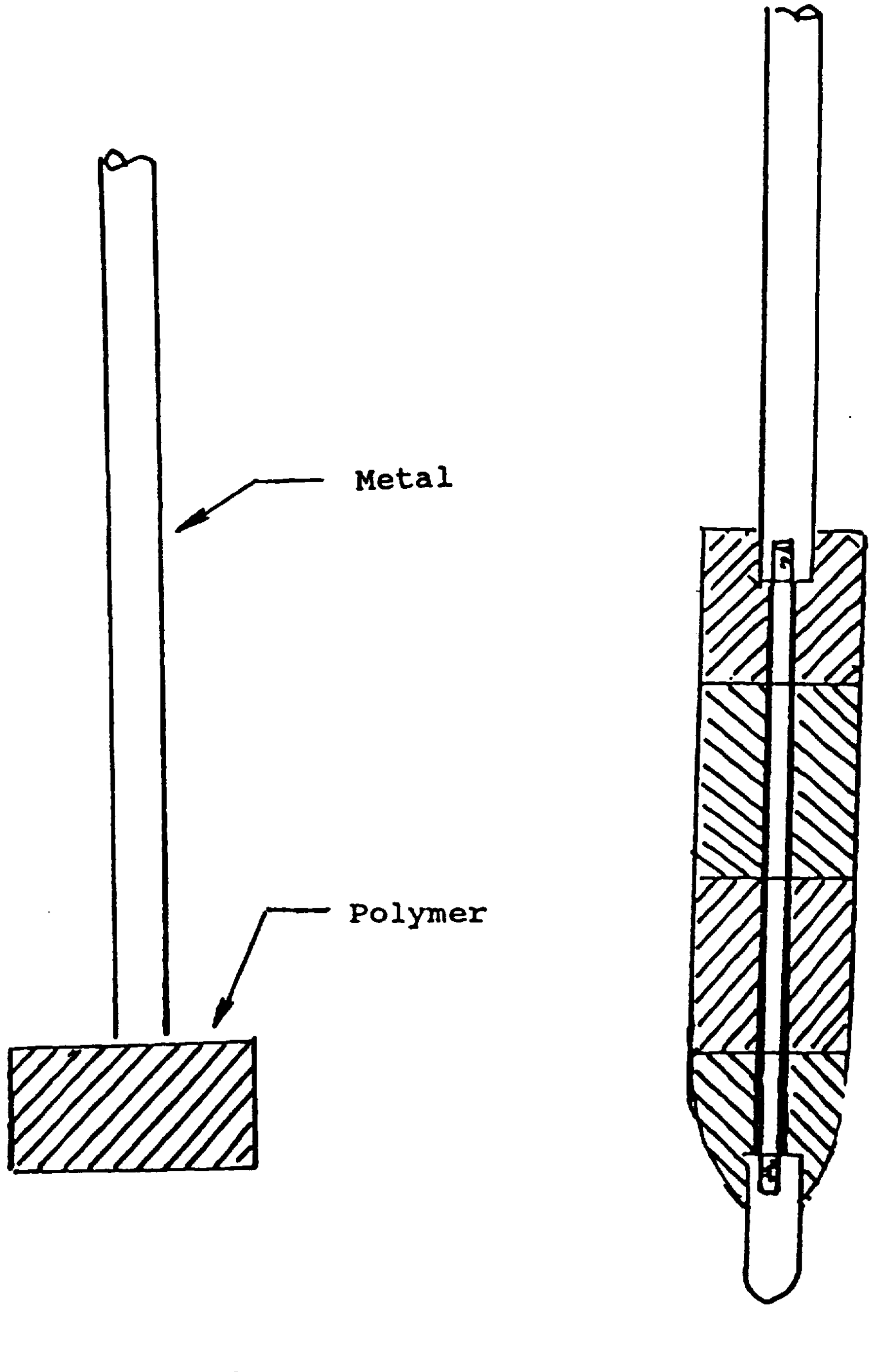


Figure 1. - Modified Test Chamber for Promoted Igntion Tests.



Current Standard

Proposed

Figure 2. - Comparison of Proposed Polymer Sample Shape with Current Standard Disk Shape.

compared in Figure 2 were calculated to have the same total burn times, assuming the surface burn rate is uniform with the disk sample. However, this estimate is considered to be inaccurate based on recent simulations made with the numerical boundary layer code STAN5 and the actual shape of the polymer required to achieve a well-defined boundary layer flow must be determined experimentally.

At a minimum, the proposed configuration provides for a convenient mathematical model to sort and analyze the effect of test configuration with an analysis of a natural convection boundary layer flow. Even the approximate integral boundary layer analysis of this flow already explains some of the different burning behavior of polyethylene and teflon observed by Shelly.

APPROXIMATE INTEGRAL BOUNDARY LAYER ANALYSIS

An approximate solution to the boundary layer equations can be obtained by integrating the equations across the thickness of the boundary layer and incorporating profile shapes for velocity and temperature. Following a procedure first used by Eckert and Jackson (1950), an integral analysis of this type was performed for assumed turbulent natural convection at the surface of a burning polymer in the proposed test configuration.

Integral Equations of the Boundary Layer

The integral equations considered are those used by Eckert and Jackson with an additional term added to the energy equation to account for convected energy at the surface due to the release of combustion products. The equations solved are:

$$-\tau_o = -g\beta\int_0^\infty \rho(T-T_\infty)dy + \frac{1}{r}\frac{d}{dx}\left(r\int_0^\infty \rho u^2 dy\right) \tag{1}$$

$$q_o'' = \frac{c_p}{r}\frac{d}{dx}\left(r\int_0^\infty \rho u T dy\right) - m_o'' c_p T_o \tag{2}$$

The radius r is constant in this application and, consequently, it does not appear in the equations actually solved.

The assumed profiles shapes for velocity and temperature are typical 1/7th power profiles for turbulent flow:

$$\frac{u}{u_1} = \left(\frac{y}{\delta}\right)^{1/7}\left[1-\frac{y}{\delta}\right]^4 \tag{3}$$

$$\frac{T-T_\infty}{T_o-T_\infty} = 1-\left(\frac{y}{\delta}\right)^{1/7} \tag{4}$$

The solution provides algebraic expressions for the boundary layer thickness δ and characteristic velocity u_1 used in these equations.

Shear, Heat Flux, and Mass Transfer at the Polymer Surface

The procedure used by Eckert and Jackson to represent surface exchange parameters τ_o and q_o'' in the integral equation was adopted. Correlations developed for forced convection are used with the free-stream velocity replaced by the characteristic velocity u_1; the resulting correlation for convective heat transfer was found by Eckert and Jackson to agreed reasonably well with experiment. Specific correlations for wall shear and heat flux are:

$$\tau_o = 0.0225 \rho u_1^2 \Psi \left(\frac{\nu}{u_1 \delta} \right)^{1/4} \tag{5}$$

$$\frac{q_o''}{\rho c_p u_1 (T_o - T_\infty)} = 0.0225 \Psi \left(\frac{\nu}{u_1 \delta} \right)^{1/4} \tag{6}$$

Here, the term Ψ is a modification to account for mass transfer at the surface; it is defined:

$$\Psi = \frac{b}{e^b - 1}, \tag{7}$$

where b is a blowing parameter,

$$b = \frac{m_o''/\rho u_1}{(C_f/2)_o} . \tag{8}$$

The denominator in Eq. (8) is the friction factor for the case of no blowing at the wall, i.e.,

$$(C_f/2)_o = \left(\frac{\tau_o}{\rho u_1^2} \right)_o . \tag{9}$$

The reader is referred to Kays and Crawford (1993) for a complete development of this correlation for turbulent forced convection with moderate surface blowing.

General power functions of the position x along the surface are assigned to δ and u_1; then, the exponents are determined by substitution of the assumed profiles and these correlations into the integral equations. The wall shear and heat flux must necessarily vary as a power of x;, and, by analogy, the mass transfer at the polymer surface must have the same power relationship. The resulting rate equations are:

$$\tau_o = F_f\, x^{0.2} \tag{10}$$

$$q_o'' = F_q\, x^{0.2} \tag{11}$$

$$m_o'' = F_m\, x^{0.2} \tag{12}$$

The constants F_f, F_q, and F_m are determined from the solutions for δ and u_1. The "carrot shape" shown in Figure 2 corresponds to Eq. (12) with the constant F_m determined for polyethylene.

Solutions for δ and u_1

The solutions for δ and u_1 are:

$$\delta = C_\delta\, x^{0.5}, \qquad u_1 = C_u\, x^{0.7} \tag{13}$$

where the constants C_δ and C_u are determined from the aforementioned substitution of profiles and correlations into the integral equations. The thermal boundary conditions and overall mass transfer rates adopted were established using measured burning rates and a convenient surface combustion model.

Surface Combustion Model

Stoichiometric combustion at the surface of the polymer is assumed for the estimated surface burning rates. The corresponding oxidant-to-fuel ratio on a mass basis is 4.51 for polyethylene and 0.32 for teflon.

Surface combustion temperatures were calculated using adiabatic flame temperatures obtained by Shelly et al. (1993) with the Gordon and McBride code (1971) and a correction for radiation losses to the chamber based on a small body in a large enclosure model. The radiation correction is:

$$Q_R = \epsilon A \sigma\left(T_o^4 - T_\infty^4\right) \tag{14}$$

Numerical Results

Table 1 presents numerical results obtained for polyethylene in oxygen at five test pressures. Four observations are:

- The flame temperatures are shown to be a strong function of test pressure; this is a result of the burning rates increasing with pressure and the radiation correction having a relatively smaller effect.

- The high flame temperatures at the higher pressures exceed the ignition temperatures of some metals.

- At all test pressures, the blowing parameter b is shown to be high in comparison to a value of 4 corresponding to "blowoff" and boundary layer separation; hence, the assumption of moderate blowing is violated and a need for a more accurate model is indicated.

- The last column is the ratio of oxidant entrained in the boundary layer to the mass of polymer burned at the surface. In all cases, this ratio is below the stoichiometric oxidant-to-fuel ratio of 4.51 and the achievement of surface combustion only cannot be met; another violation of a model assumption. However, this result is corroborated by the data of Shelly et al. where a wide diffusion flame with combustion in the boundary layer was observed.

TABLE 1. - RESULTS OF INTEGRAL BOUNDARY LAYER CALCULATIONS.

P (Mpa)	T_f (K)	C_δ	C_u	b	m_e''/m_o''
3.4	2022	0.1034	4.8673	3.48	3.48
6.9	2204	0.0805	4.5150	2.87	3.24
20.4	2610	0.0636	4.5969	2.60	3.32
34.4	3043	0.0751	4.7239	3.63	3.11
68.9	3294	0.0565	4.7304	1.60	3.25

The assumption of turbulent natural convection was confirmed by the calculated Grashof numbers Gr_x at x equal to 10 mm. Values range between 10^6 at the lowest test pressure to 10^{11} at the highest test pressure.

Velocity and temperature profiles constructed from these numerical results vary in both magnitude an extent beyond the polymer surface as the boundary layer develops. It follows that different thermal and flow conditions can be achieved at the interface of the polymer and metal rod samples by simply extending the length of the polymer test sample.

Numerical results were not obtained for teflon. However, the mass ratios for teflon are expected to be comparable to those calculated for polyethylene and the achievement of a stoichiometric mass ratio of 0.32 at the surface is considered quite feasible. This result is also corroborated by the observations of Shelly et al. where near surface combustion was observed with the teflon samples.

STAN5 - A NUMERICAL COMPUTER MODEL

The inability to validate model assumptions made in the integral analysis indicated that a more detailed model accounting for combustion in the boundary layer flow is needed. The computer code STAN5, previously developed for NASA by Kays et. al. [Julien (1969, 1971), Kays and Crawford (1976)] at Stanford University, was acquired from the NASA Lewis Research Center for this purpose. It is a version of a general purpose boundary layer calculation code developed by Patankar and Spaulding [Patankar and Spaulding (1967, 1970), energy and the diffusion equations for any number of species; in particular, the equations solved are:

$$\frac{\partial}{\partial x}(r\rho u) + \frac{\partial}{\partial y}(r\rho v) = 0 \tag{15}$$

$$\rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} = g_c X - g_c\frac{dP}{dx} + \frac{1}{r}\frac{\partial}{\partial y}\left[r \left(\mu\frac{\partial u}{\partial y} - \rho\overline{u'v'} \right) \right] \tag{16}$$

$$\rho u\frac{\partial i*}{\partial x} + \rho v\frac{\partial i*}{\partial y} = \frac{1}{r}\frac{\partial}{\partial y} \left(r \left[\frac{k}{c}\frac{\partial i*}{\partial y} - \rho\overline{i*'v'} + \sum_j \gamma_j \frac{\partial m_j}{\partial y} i_j + \frac{\mu}{g_c J}\frac{\partial}{\partial y}\left(\frac{u^2}{2}\right) \right] \right) + \frac{uX}{J} \tag{17}$$

$$\rho u\frac{\partial m_j}{\partial x} + \rho v\frac{\partial m_j}{\partial y} = \frac{1}{r}\frac{\partial}{\partial y}\left(r \left[\gamma_j\frac{\partial m_j}{\partial y} - \rho\overline{v'm_j'} \right] \right) + \dot{m}_j''' \tag{18}$$

This computer program has been installed on both the WSTF and NMSU computer systems in preparation for future more detailed analysis. Test runs have been made and some initial modeling of boundary layer flows on a burning polymer sample has been accomplished; but, combustion in the boundary layer flow and species transport were not considered.

The analysis of the boundary layer flow with combustion does require detailed thermodynamic data for the test polymers. To obtain these data, a test program involving the use of a cone-calorimeter developed by Hshieh et. al. (1993) is being considered as a possible parallel research activity at WSTF.

CONCLUSIONS

1. The revised promoted combustion tests should provide for the evaluation of configuration specific parameters on test results. Different thermal and flow conditions can be achieved near the metal sample by simply changing the length of the polymer sample in the new test configuration.

2. An approximate integral boundary layer analysis demonstrated the capability to evaluate configuration specific parameters in the revised test and did explained some of the visual test observations made by Shelly et. al. in recent promoted combustion tests. However, basic assumptions of moderate mass injection and stoichiometric combustion at the polymer surface were found not to be valid.

3. A numerical boundary layer prediction code STAN5 has been made available and it is capable of analyzing more accurately and in greater detail the revised promoted combustion tests. And the required thermodynamic data to address combustion within the boundary layer flow can be obtained in a parallel test program at WSTF.

RECOMMENDATION

Continuation of this research activity through Academic Year 93/94 and Summer 1994 is recommended. This should be accomplished in parallel with the test program to obtain requisite thermodynamic properties of polymers. And, it should be followed by the modification of the test chamber and development of the revised promoted ignition test.

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