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ON EXHAUST HYDROCARBON EMISSIONS

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## TABLE OF CONTENTS

PREFACE	1
1. INTRODUCTION	2
2. RECENTLY REPORTED RESULTS	3
3. MODELING OF ONE-WALL AND TWO-WALL QUENCHING	5
REFERENCE	9
FIGURES	10
APPENDIX A. NONISOBARIC FLAME PROPAGATION	13
APPENDIX B. CYCLIC ABSORPTION/DESORPTION OF GAS IN A LIQUID WALL FILM	33

## PREFACE

Technical review of this project was carried out by C. William Robinson, Combustion Applications Division, Sandia Laboratories, Livermore, California.

The work reported in this document was carried out by George Carrier (consultant), Francis Fendell (principal investigator), and Phillip Feldman. The participants wish to thank Warren Ferguson for his advice and contribution with respect to the numerical analysis.

## 1. INTRODUCTION

This project is concerned with simple modeling and laboratory experiments to elucidate (1) the mechanisms whereby trace amounts of unburned hydrocarbons may persist after the combustion event in Otto-cycle-type internal-combustion-engine cylinders, and (2) the fate of these residual hydrocarbons during the power-stroke and exhaust-event portions of the cycle. The motivation for the research is that a highly fuel-lean fast-burn design for the spark-ignition homogeneous-charge, four-stroke engine may permit exceptionally fuel-efficient operation of this highly driveable, relatively well-understood automotive engine. Without such operation, the long-term prospects for continued utilization of the Otto-cycle engine are uncertain. However, augmented unburned-hydrocarbon content of the cylinder exhaust gas may occur under fuel-lean stoichiometry; such emissions are environmentally objectionable because some hydrocarbons are suspect as carcinogens and/or as participants in smog formation. Thus insight to guide design alternatives to remove the unburned-hydrocarbon liability is of current concern to automotive engineers.

As reviewed in the final technical report to Phase 4 of this program (TRW 1980), there are three likely mechanisms that leave residual unburned hydrocarbon vapor: quenching of flame propagation near engine cylinder walls maintained relatively cold for material integrity (one-wall quenching); failure of flame to propagate into narrow crevices near the piston rings and spark plugs (two-wall quenching); and cyclic absorption/desorption of hydrocarbons into/from the thin oil film coating the lateral surface and piston crown owing to reciprocating-piston motion. Because all three just-listed mechanisms are being pursued in this project under severe funding restraints, other mechanisms (failure of a spark kernel to form owing to mixture inhomogeneity, failure of bulk-gas burn-up owing to reduced flame-propagation speed in off-stoichiometric mixtures) are not considered within the domain of investigation.

## 2. RECENTLY REPORTED RESULTS

In Appendix A of this report is a discussion of nonisobaric unsteady flame propagation through a homogeneous premixture confined between plane parallel impervious walls. The enclosure encompasses constant total mass, but is of variable volume, because one wall is permitted to move to simulate piston motion. The work is of interest in itself because it encompasses a suggestion with respect to modeling of turbulent flame propagation, a suggestion based on recent observations in bombs of persistent coherent structure in a flame zone (of finite thickness) that separates virtually fully unburned from virtually fully burned gas. Specifically, the enhanced rate of flame propagation of the turbulent case relative to the laminar case is owing to enhanced areal exposure of unburned gas to burned gas. The consumption rate is the same per unit length of the flame (which may be, and probably is, multiply connected) as in the laminar case; i.e., the laminar flame speed based on the local properties of the particle being engulfed is locally pertinent (both spatially and temporally). The enhancement in conversion of reactant to product is owing to the ever-increasing convolutions experienced by the flame undergoing straining in a highly nonuniform flowfield. (The enhancement never becomes unboundedly large, and one suspects a "flame-shortening" mechanism would eventually counterbalance the "flame-stretching" mechanism, as more and more flamelets compete for less and less fuel.)

The motivation for undertaking the work reported in Appendix A is really as a first sally into what is to become a dominant subject of investigation in future research: the effectiveness of burn-up of residual fuel vapor during the power stroke, during which expansional cooling occurs. The temporally variant pressure alters the entropy of the system directly, but also through the pressure dependence of the diffusion coefficients and the reaction rate. Thus, while there is excess oxygen-rich hot bulk gas available to consume any residual near-wall hydrocarbon vapor, the completeness of the burn-up warrants scrutiny.

In Appendix B, the cyclic nature of absorption and desorption of unburned hydrocarbon gas in the thin near-wall oil layer left on the

lateral surface of the cylinder owing to reciprocating-piston motion (and splashed onto the piston crown) is examined for fuel-lean stoichiometry (only). For oil layers as thick as 10 microns (and measurements indicate such thicknesses are attained), diffusional resistance of the oil film to absorption of the vapor is rate-controlling. The significant decrease (by a factor of four) of unburned HC content (from, say, 2000 ppm concentration to 500) as the rpm is increased from 1500 to 3000 is explicable in terms of oil-layer effects, whereas the decrease of exhaust content with increasing engine speed is inexplicable in terms of one-wall and/or two-wall quenching mechanisms. However, if the oil film is but a micron thick, the film saturates with hydrocarbon-vapor content at almost any engine speed of practical interest; diffusional resistance of the oil film is not rate-controlling and the explanation for the decrease of unburned HC content in cylinder exhaust gas appears not to be furnished by oil-film effects.

It may perhaps be worth noting that decrease of unburned hydrocarbon content (say, by a factor of 2) of the exhaust gas with a modest increase in coolant temperature (say, from 320 K to 380 K) cannot be explained in terms of one-wall or two-wall quenching. (While the cooling temperature need not be identical to the wall temperature, there is a rapid adjustment such that the temperature of one may well be indicative of the temperature of the other.) However, the increment in Henry's constant with increasing temperature is so great that perhaps reduced oil-film absorptivity is a possible explanation. (For thermodynamic equilibrium, Henry's constant is inversely proportional to the mole fraction of vapor in the liquid, for very dilute solution, the vapor pressure of the solute in the gas phase being held constant.)

### 3. MODELLING OF ONE-WALL AND TWO-WALL QUENCHING

Both the unsteady, one-dimensional, parabolic problem of a premixed flame approaching a parallel planar impervious noncatalytic isothermal wall, and also the steady, two-dimensional, elliptic problem of a burner-stabilized premixed flame situated perpendicular to a planar impervious noncatalytic isothermal wall, have been examined in detail in this project. The former arrangement is alluded to as "head-on quenching" for an "end-wall geometry"; there is virtually no existing experimental data concerning flowfield details. The latter arrangement is alluded to as the "side-wall geometry", and the first experimental flowfield details via nonintrusive modern diagnostic optical techniques (specifically, by laser Raman spectroscopy) were also obtained in this project.

Here attention is confined to reporting modeling results for the side-wall geometry, obtained by numerical integration of a Shvab-Zeldovich formulation via ADI techniques. A so-called Shvab-Zeldovich formulation incorporates the essential physics in tractable equations preserving engineering accuracy. In particular, a direct one-step bimolecular reaction of Arrhenius type, with universal diffusion coefficient (of simplistic thermodynamic dependence) and Lewis-Semenov number unity and comparable molecular weight for all species present, is adopted; the flowfield for the convective transport of heat and mass is prespecified, and mechanical dissipation, radiative transfer, and thermodiffusion and barodiffusion are ignored. This formulation still leaves two coupled, transcendently nonlinear elliptic partial differential equations with interior-boundary-layer-type behavior.

In this reporting period, a strenuous effort was expended, to no avail, to apply multigrid methods to the boundary-value problem. These techniques use point-type methods, with Gauss-Seidel-type iteration, on a series of grids of varying resolution, to relax as required the low-frequency and high-frequency components of the residual generated by substitution of a guessed solution. Multigrid methods have been effective on linear elliptic problems with Dirichlet boundary conditions, and even on mildly (algebraically) nonlinear equations. However, Neumann boundary

conditions appear to retard the relaxation to a solution, but, more significantly, at its present stage of development, the method in a finite-difference form appears unable to cope with large gradients characterizing the presence of a vigorous, exothermic flame (of narrow but finite structure) in a larger convective-diffusive flowfield. While future evolution of multigrid concepts in a finite-element methodology may prove effective, currently only the line-type methods (combined with quasilinearization and block inversion) seem readily able to cope with the side-wall quench layer.

In this reporting period emphasis was placed on obtaining results for a Blasius-type flowfield (enforcing no-slip boundary conditions on the quench plate), as opposed to the previously employed Oseen-type flowfield (permitting perfect slip at the quench plate). For the eigenvalue problem associated with flame propagation between planar, parallel, impervious, isothermal (cold), noncatalytic walls, for the Blasius-type flowfield convergence of the iterations proved too slow and costly to be pursued. Thus the reduction of flame speed with approach of the plates, previously obtained under an Oseen flowfield, still remains the only results computed to date with a Lewis-Semenov number of a value pertinent to hydrocarbon/air premixtures. However, for the one-wall problem (i.e., for separation distance so large that the presence of a second plate, if any, is academic, and (nominally) a prespecified one-dimensional flame structure -- as opposed to a centerplane symmetry condition -- becomes the boundary condition applied away from the side wall), results could be obtained for a Blasius-type flow. Even in the one-wall case, imposition of the Blasius-boundary-layer solution in the convective transport required compromise, as now reported.

The effect of the no-slip-type flow so increased the thickness of the wall-quench layer that even roughly comparable grids in the streamwise and transverse directions became impossible. Since one wishes to adopt comparable grids for numerical accuracy, the procedure adopted was to enforce no more than a Neumann-type (as opposed to a Dirichlet-type) boundary condition on the fuel mass fraction and on the temperature away from the side wall. More explicitly, instead of enforcing a precalculated one-dimensional flame structure as the outer boundary condition for the

quench layer solution, the solution was free to develop its own outer structure, within the constraint of vanishing normal derivative. It turns out that the outer flame structure generated under a Neumann constraint is virtually what would have been imposed under a Dirichlet constraint, except that the flame is displaced about one-quarter diffusive scale (about 0.003 cm) downwind.

Although evaluation of the recently achieved computational results is still highly incomplete, some presentation for the single-side-wall steady two-dimensional laminar quench layer under a Blasius-type flow-field is undertaken. The following terminology is introduced. The streamwise coordinate  $x$  is measured from the leading edge of the quench plate (placed against the porous-sintered-bronze disc of the flameholder face); the transverse coordinate  $z$  is measured from the quench plate. Both  $x$  and  $z$  are nondimensionalized against the diffusive scale mentioned in the last paragraph; the diffusive scale characterizes the thickness of the preheat zone in premixed-flame structure (for large-Arrhenius-activation-temperature hydrocarbon/air premixtures), and is the ratio of the mass transfer coefficient in Fick's law (evaluated in the cold gas) to the adiabatic laminar flame speed. The stoichiometrically adjusted mass fraction for fuel, normalized to the value unity in the unburned gas issuing from the burner, is denoted  $Y$ . The selfsimilar factor in the streamfunction for laminar isobaric flow past a long flat plate, the so-called Blasius function, is denoted  $f'$ , and  $f'_w$  signifies  $f'$  evaluated at  $z = 0$ , i.e., at the quench plate surface. The value  $f'_w = 1$  denotes no retardation at the wall relative to the streaming away from the way (perfect slip), whereas the value  $f'_w = 0$  denotes no motion at the wall relative to the wall (zero slip). The transversely integrated mass fraction  $I(x)$  is defined as follows:

$$I(x) = \int_0^{\infty} Y(x,z) dz;$$

the mass flux fraction  $J(x)$  is defined as follows:

$$J(x) = \int_0^{\infty} \rho(x,z) u(x,z) Y(x,z) dz.$$

For perfect slip ( $f'_w = 1$ ),  $\rho(x,z)u(x,z) \equiv 1$  for all  $x,z$ , such that  $I(x) = J(x)$ ; for no-slip conditions ( $f'_w = 0$ ),  $I(x) \neq J(x)$ . The case ( $f'_w = 1$ ) is alluded to below as the nominal case.

Figure 1 reveals, by comparison of constant-mass-fraction lines, that the quench-layer thickness is appreciably greater for the Blasius-type flowfield (no slip) than for the Oseen-type flowfield (perfect slip). Other parameter values are not explicitly called out because they remain invariant under the parametric comparisons explicitly noted. However, for completeness, the fuel-lean burning of a simple hydrocarbon in air under low-speed isobaric conditions is being considered.

Figure 2 reveals that, while the fractional amount of original fuel that persists unburned in the quench layer is somewhat greater in the no-slip case, by about eight diffusive scales downwind the differences are of negligible consequence for most purposes.

Figure 3 presents the outer mass-fraction-profile as a function of streamwise distance (obtained from a one-dimensional solution of the flame structure) that is impressed as an outer boundary condition in Oseen-type (perfect-slip) calculations. Also presented is the outer mass fraction profile as a function of streamwise distance (evolved) as part of a two-dimensional solution of the quench layer) that is obtained from the zero-normal-gradient outer boundary condition used in Blasius-type (zero-slip) calculations. The discrepancy consists, more or less, of a modest streamwise displacement.

## REFERENCE

TRW Defense and Space Systems Group, 1980. Wall quench and flammability limit effects on exhaust hydrocarbon emissions--final technical report, phase 4. TRW Report 32512-6002-RU-00, 17 pp. Redondo Beach, CA: Engineering Sciences Laboratory.

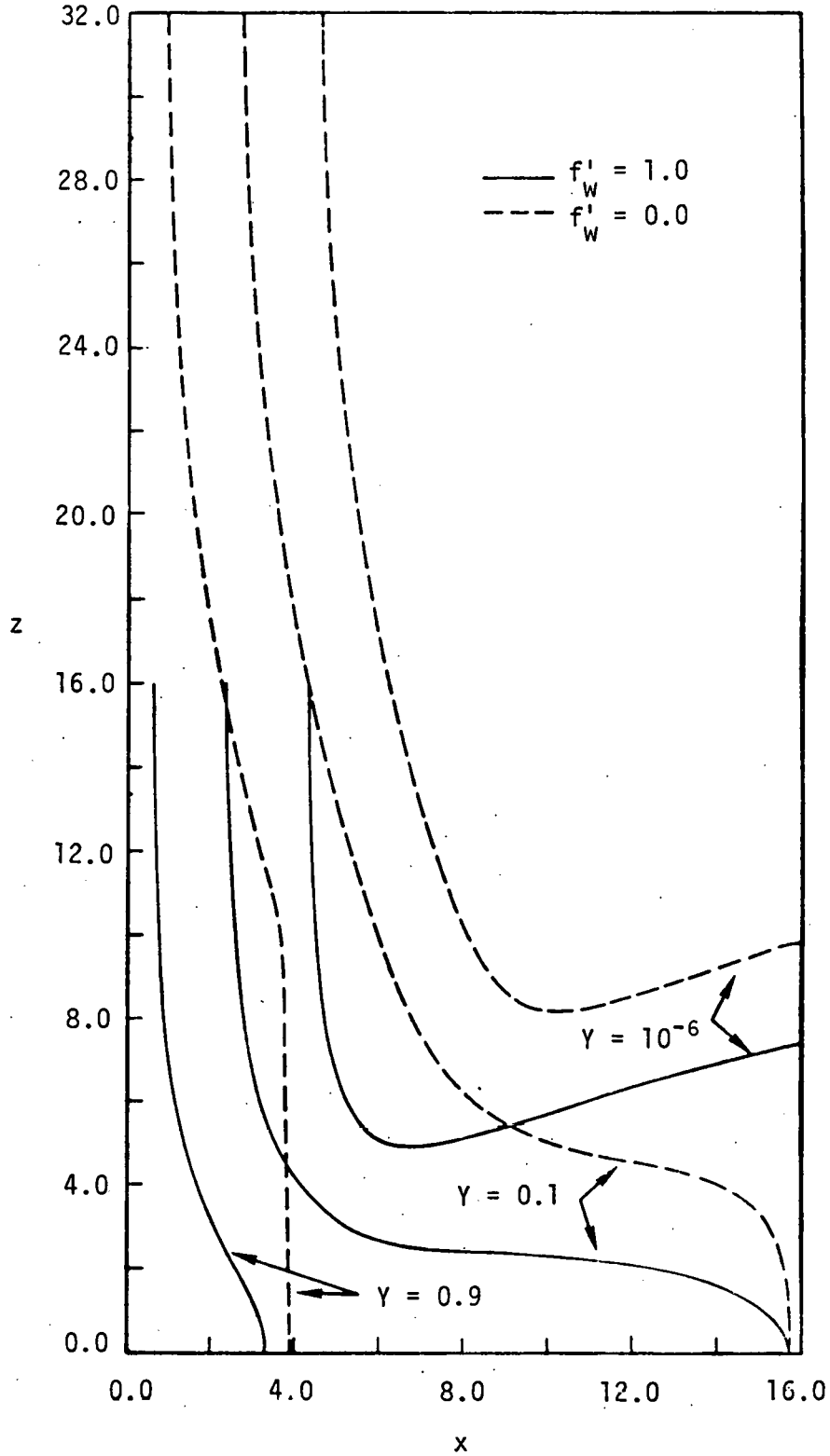


Figure 1. Constant-mass-fraction surfaces for a cold impervious noncatalytic side wall are compared for the nominal case (slippery wall  $f'_w = 1.0$ , Dirichlet outer condition) and the no-wall-slip case ( $f'_w = 0.0$ , Neumann outer condition).

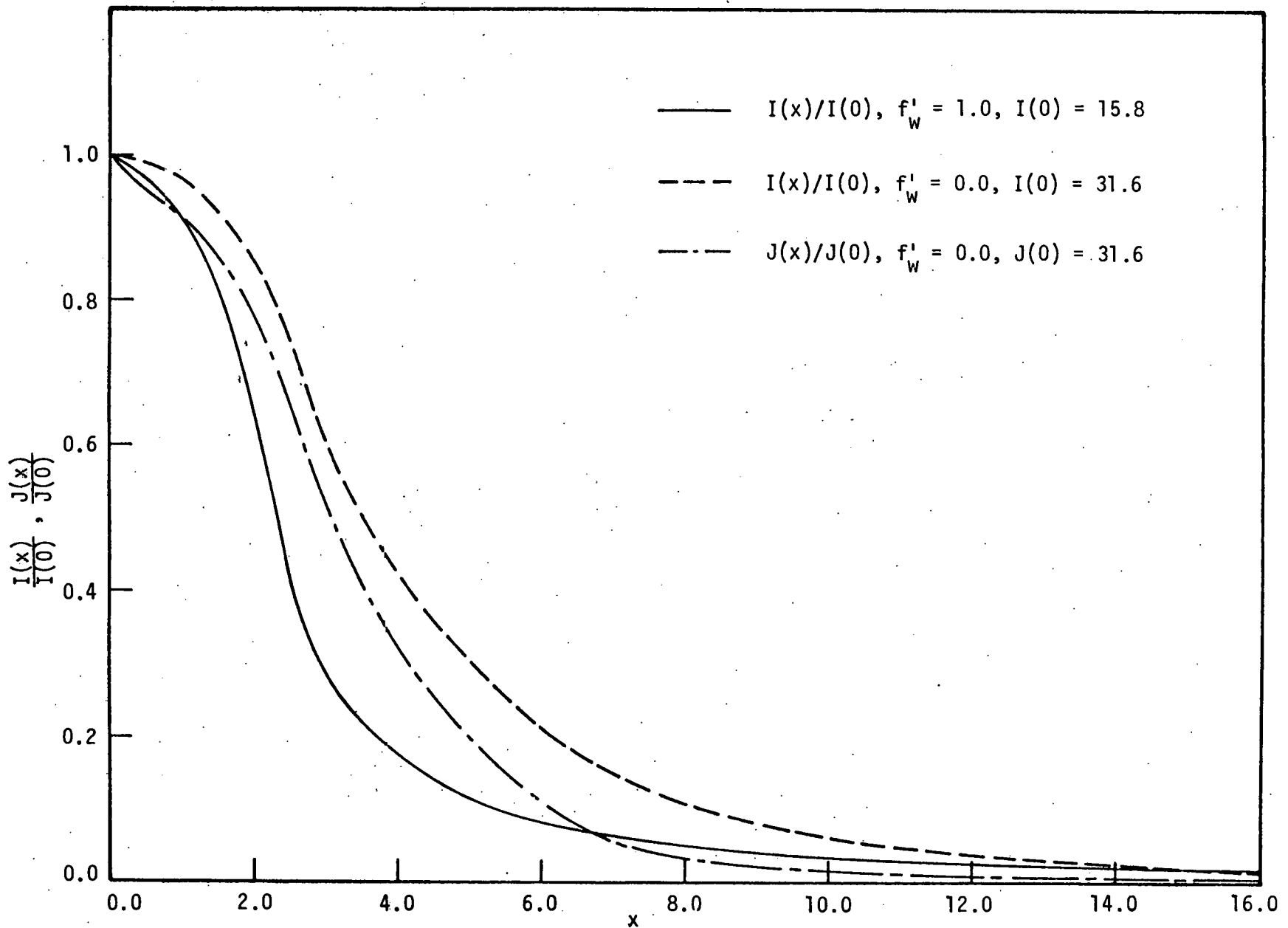


Figure 2. The ratio of the transversely integrated normalized fuel mass fractions  $I(x)$ ,  $J(x)$  to their values at the leading edge  $I(0)$ ,  $J(0)$ , given as a function of streamwise distance  $x$  for the nominal slippery-wall case ( $f'_w = 1$ ) and for the case of no wall slip ( $f'_w = 0$ ). For the nominal case,  $I(x) = J(x)$ .

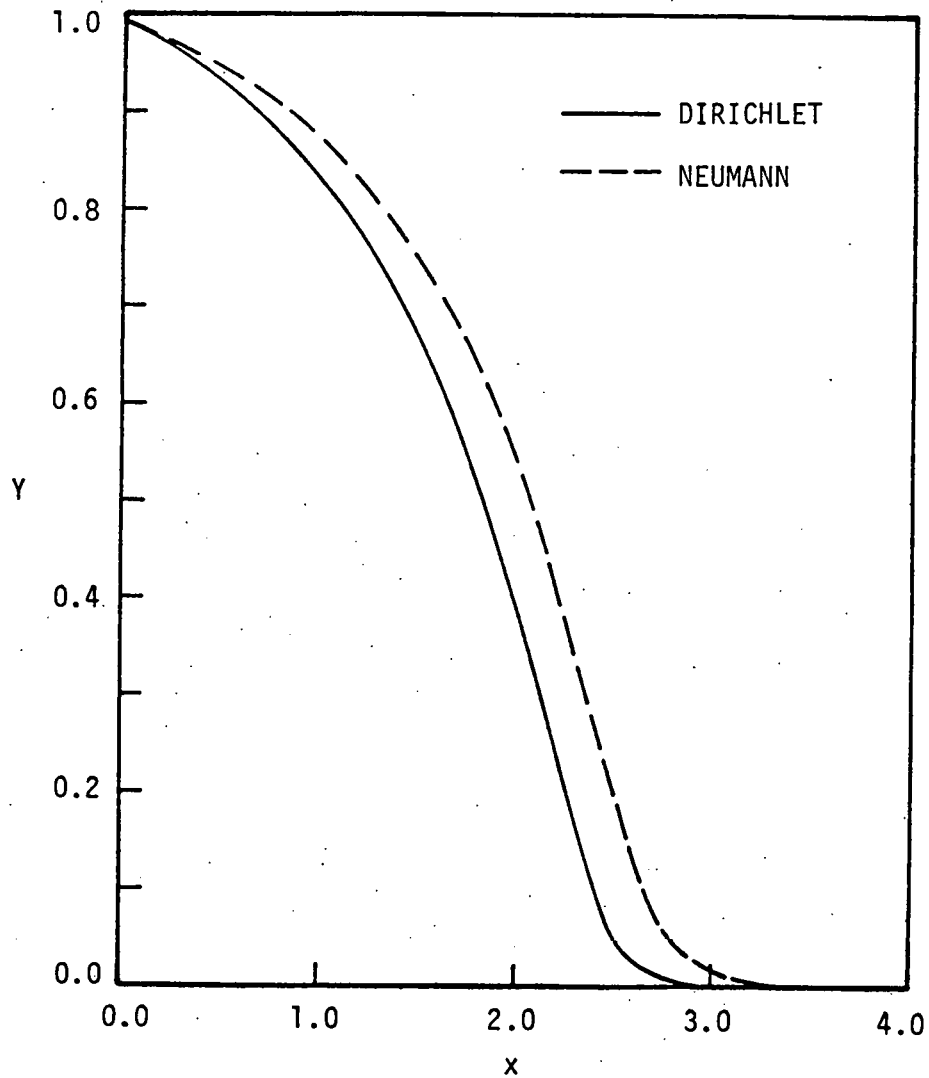


Figure 3. A comparison is presented of mass-fraction profiles at the outer  $z$  boundary for the case  $f_w' = 0.0$ ,  $z_{\max} = 32.0$  with a Dirichlet boundary, and for the case with a prescribed Neumann boundary.

APPENDIX A

NONISOBARIC FLAME PROPAGATION

by

George F. Carrier, Francis E. Fendell, and Philip S. Feldman  
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Errata

- page 334, eq. (2.2)      the upper limit of the integral  
should be  $\psi$ , not  $x$ .
- page 338, eq. (2.16)    the denominator of the last factor  
on the right-hand side should be  $p$ ,  
not  $P$

*reprint  
removed*

APPENDIX B

CYCLIC ABSORPTION/DESORPTION OF GAS IN A  
LIQUID WALL FILM

by

George Carrier, Francis Fendell, and Phillip Feldman

27 pp.

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