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Volume II



**LEVEL III**

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# EDLAMP USER'S MANUAL

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Prepared for

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Repetitively Pulsed Laser Electric Discharge Plasma Chemistry Electrophilic Species		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)		
A computer program is described which can be used to analyze plasma chemistry effects on the performance of pulsed, electron-beam sustained, electric discharge lasers operating either in the open cycle or closed cycle mode.		

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## FOREWORD

This report presents results of work performed by the Lockheed-Huntsville Research & Engineering Center under Contract DAAH40-78-C-0196, for the U.S. Army Missile R&D Command, Redstone Arsenal, Alabama.

This work was jointly monitored by Mr. Charles M. Cason, Chief, Electric Laser Branch, Army High Energy Laser Center (Prov.), and Capt. John Filcoff of the Electric Laser Branch, Air Force Weapons Laboratory. The period of performance covered by this report was from 5 July 1978 through 5 July 1979.

This is Volume II of a two-volume report.

- "Plasma Chemistry Processes in the Closed Cycle EDL," Volume I - AOS3222
- "EDLAMP User's Manual," Volume II.

The present document replaces the previously issued EDLAMP User's Manual, Technical Report H-CR-77-7, Vol. II, January 1977.

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## 1. INTRODUCTION

The purpose of this document is to present the user's information needed to exercise the Electric Discharge Laser and Mixing Program (EDLAMP). This program is particularly suited to investigate plasma chemistry processes in electric discharge lasers. The output power under lasing conditions can be predicted fairly well although the validity of intensity distributions is constrained by the use of a "constant gain" radiation calculation and the assumption of an oscillator with plane parallel mirrors (Fabry-Perot cavity). The code can model both pulsed and continuous wave lasers, under either open cycle or closed cycle operation.

The EDLAMP code is a direct derivative of the Lockheed LAMP code (Ref. 1) and therefore retains capabilities such as the two-dimensional flow field and viscous mixing calculations. Although EDL calculations presently are restricted to one-dimensional calculations (the independent coordinate is either time, or distance along the direction of flow) because the effects of both electron beam and electric discharge are modeled in terms of average quantities that depend only on either time or distance along the flow, the two-dimensional coding was retained with a view toward future refinements of the analysis of electric discharge laser cavities.

Proper use of the EDLAMP code requires knowledge of certain quantities such as drift velocity and electron impact excitation rates. This information is obtained from a Boltzmann code. It is therefore deemed appropriate to also present in this volume the information needed to exercise the Boltzmann code (Ref. 2).

Section 2 presents a brief technical discussion of the options available to the EDLAMP and Boltzmann code user, while Section 3 contains the actual guide for both codes.

## 2. TECHNICAL DISCUSSION

### 2.1 GENERAL INFORMATION

The Boltzmann code used here is specifically designed for the analysis of CO<sub>2</sub> lasers. The code can handle up to nine five-component gas mixtures. Cross-section data are provided for CO<sub>2</sub>, N<sub>2</sub>, He, H<sub>2</sub>, CO, and O<sub>2</sub>. Results of this code are used in the EDLAMP code in terms of curve fits for the drift velocity as a function of E/N, and in terms of curve fits for the impact excitation rates as a function of average electron energy. While fitting the drift velocity is straightforward, fitting the impact excitation rates is somewhat more laborious, less so with a little experience. The main reason for fitting the impact rates as a function of the average electron energy is that it renders these, at least the vibrational excitation rates, practically insensitive to gas mixture variations. Checks should be made before using already fitted rates for new mixtures. Scaling with average electron energy is not as good for electronic excitation and ionization rates, except for minor variations in laser gas mixtures. The Boltzmann code is a fast running program, but requires considerable amounts of central memory which renders direct coupling with the EDLAMP code impractical.

The EDLAMP input deck consists of 32 cards (or card groups). Some of these cards may be omitted depending on the problem to be investigated. The problem choice is determined entirely by the values of a number of "flags" contained on cards 2 through 5. Geometric data for flowing gas continuous wave laser calculations (or equivalent times for pulsed laser calculations) are set on cards 6 through 8. Card group 9 specifies the characteristic data for the electron beam and the electric discharge, as well as the curve fit coefficients for the drift velocity as computed from the Boltzmann code output. For the investigation of closed cycle laser operation, card group 10 specifies integration step sizes to be used in the cycle simulation, catalyst contaminant

removal efficiencies for each species, leak and laser gas makeup rates as well as their respective constituents. Cards 11 through 14 specify the flow problem in terms of initial values for the gas composition, flow velocity, temperature and grid setup. Cards 15 through 18 contain data for turbulent flow calculations which presently do not apply to EDL analyses. Cards 19 through 21 are used to specify thermodynamic properties, reaction mechanisms and rate constants. The information needed to calculate lasing performance is specified on cards 22 through 27. Cards 29 through 31 are used to specify pressure and/or temperature throughout certain regimes of the calculation. Card 32 contains parameters for the grid point control scheme which only applies to two-dimensional flowfield calculations.

In the remainder of this section detailed guidelines will be given for setting up either pulsed or continuous wave EDL calculations. In both cases options exist to do plasma chemistry calculations only, with or without the effects of recirculation. Note that quantities specified in the EDLAMP input guide as distances along the flow direction are to be interpreted as time intervals for pulsed calculations.

Any rate calculations, regardless of the program option used, require specification of reaction type and rate constant type (see card 21.1). The following rules apply:

	<u>Reaction</u>		<u>Type</u>
A + B	$\rightleftharpoons$	C + D	(1, 7)
A + B + M	$\rightleftharpoons$	C + M	(2, 8)
A + B	$\rightleftharpoons$	C + D + E	(3, 9)
A + B	$\rightleftharpoons$	C	(4, 10)
A + M	$\rightleftharpoons$	C + D + M	(5, 11)
A + M	$\rightleftharpoons$	C + M	(6, 12)
A(v) + e	$\rightarrow$	A(v') + e	(13)
A + e <sub>EB</sub>	$\rightarrow$	A <sup>+</sup> + e + e <sub>EB</sub>	(14)
A + e <sub>EB</sub>	$\rightarrow$	A* + e <sub>EB</sub>	(15)

Reaction types (7) through (12) correspond to reaction types (1) through (6), but proceed in the forward direction only.

<u>Rate Constant</u>	<u>Type</u>
$k_f = A$	(1)
$k_f = A T^{-N}$	(2)
$k_f = A \exp(B/\mathfrak{R} T)$	(3)
$k_f = A T^{-N} \exp(B/\mathfrak{R} T)$	(4)
$k_f = A T^{-N} \exp(B/\mathfrak{R} T^M)$	(5)
$k_f = A \exp(B/u_e)$	(6)
$k_f = \frac{A u_e^{-N} \exp(B u_e)}{1 + A_1 u_e^{-N_1} \exp(B_1 u_e)}$	(7)
$k_f = \frac{A u_e^{-N} \exp(B/u_e)}{1 + A_1 u_e^{-N_1} \exp(B_1/u_e)}$	(8)
$k_f = A u_e^{-N} \exp(B/u_e)$	(9)
$k_f = A T^{-N} u_e^{-M}$	(10)

Rate constants types (6) through (10) are used to curve fit impact excitation rates obtained from the Boltzmann code. For further details the user should consult the following subsections. Complete reaction mechanisms and rate constants are available in Vol. I of this report.

## 2.2 PULSED LASER CALCULATIONS

It is assumed that the user is familiar with the theoretical model upon which these calculations are based (Vol. I). In this subsection specific details on how to use the EDLAMP input guide will be given for all input parameters which are not self-explanatory in the input guide.

Card 2: According to the underlying assumptions, set MPSI = 3, NTYPE = 1, ITURB = 0.

For single pulse calculations set IPRESS = 1, ITYPE = 0, KBL = 0.

For repetitively pulsed discharges with recirculation, the above three flags are used to read the pressure distribution during the adiabatic expansion following the pulsed discharge, and the temperature distribution in the recirculation duct (in order to simulate the effects of heat exchangers). Therefore, in this case set IPRESS = 0, ITYPE = 1, KBL = 1. At the end of the input routine all three flags will automatically be reset to 1, 0, 0, for the pulse, and to 0, 1, 0 for the remainder of the cycle, respectively. Figure 1 will clarify this arrangement.

NM designates the number of catalytic species used in three-body reactions. For reasons of program logic, primary electrons are treated like a "third body" species named "EB." Therefore, the last of the NM catalytic species to be input according to card group 20 must be called "EB," and have zero weighting factors for all NS species.

Card 4: For pulsed discharges, the JRAMP flag controls the post-foil electron beam current density as a function of time during the pulse ( $XEB \leq t \leq EBLEN$ ); if EBJ (see card 9) is supposed to be constant, set JRAMP = 0, or omit; if JRAMP = 1, the effective post-foil E-beam current density will, for each pulse, vary linearly from zero at XEB to EBJ at EBLEN (see card group 8; also note Section 2.3).

Some of the plasma chemistry reactions (Vol. I) are extremely fast, necessitating extremely small integration step sizes if explicit integration of the rate equations is used. Therefore always use the implicit chemistry routine, i.e., set IMP = 1.

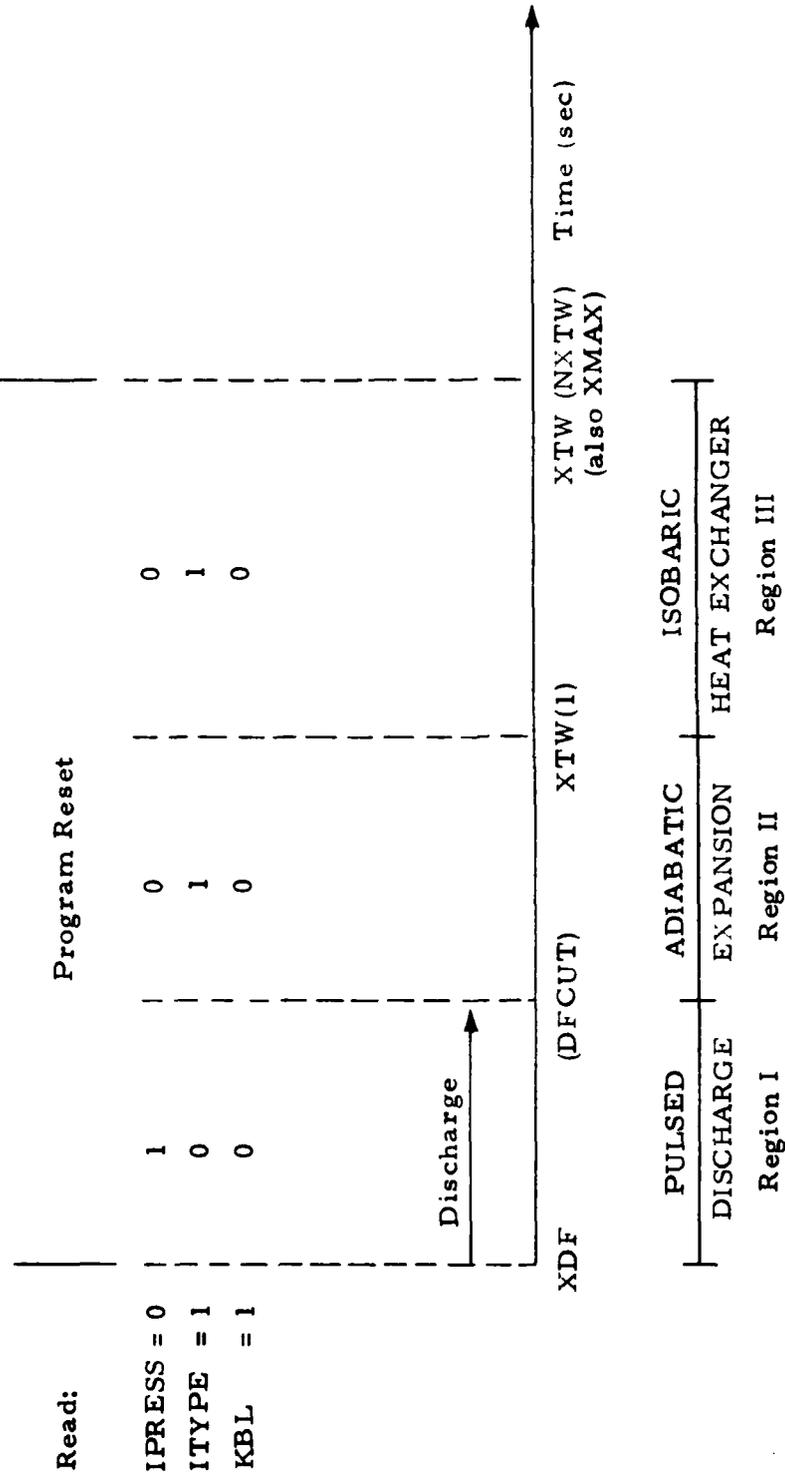


Fig. 1 - Recirculation Loop Control Flag Setup for IPRESS, ITYPE and KBL

Card 5: Under the present assumptions the laser gas is assumed to be inviscid, therefore, set  $XK2 = 0.0$ ; for reasons of coding logic set both  $XLE(1)$  and  $SIGMA(1)$  to unity.

Card 6: For pulsed discharge calculations all parameters through column 60 are entered as time intervals (sec). Parameters  $CXD$  and  $CDX$  are only used in combination with explicit chemistry calculations, and can therefore be omitted.

Card 8.1: Similar to card 6,  $XEB$ ,  $EBLEN$ ,  $XDF$  and  $DFLEN$  designate time intervals (sec);  $YDRF$  is used to evaluate the electric field and should be entered as a distance regardless. For pulsed discharge calculations set  $THETA = 0.0$ .

Card 8.2: For pulsed discharge calculations set  $ACAV = 0.0$ ; assuming that the electron beam and the discharge pulse are initiated at the same time ( $X = 0.0$ ), set  $XCAV$  equal to the larger one of  $EBLEN$  and  $DFLEN$ ; set  $XSTART \geq XMAX$ .

Card 12: The input values for  $U(I)$  are arbitrary and, for pulsed discharge calculations, will be set to unity internally (which serves to convert the spatial convective derivative into a time derivative).

Similarly, input values for  $Y(I)$  are arbitrary, however, non-zero values must be entered for  $Y(I > 1)$ . It is suggested that  $Y(1) = 0.0$ ,  $Y(2) = 0.5$  (RJ), and  $Y(3) = RJ$  (see card 5).

### 2.3 CONTINUOUS WAVE LASER CALCULATIONS

The only fundamental difference between the one-dimensional theoretical models for pulsed discharge lasers and continuous wave discharge lasers concerns the interpretation of the independent variable, which is time in the former, and the spatial coordinate along the flow direction in the latter.

The continuous wave electric discharge laser model inherent in EDLAMP differs from the model previously developed (Refs. 3, 4) in the modeling of the laser radiation field. While the model described in Refs. 3 and 4 makes use of a Fresnel integral diffraction calculation, the EDLAMP code treats radiation via a simpler, geometric optics model (Fabry-Perot cavity) using a constant gain radiation model.

In developing the pulsed discharge model care was taken not to destroy the previously developed capability to model continuous wave discharge lasers, however, time did not permit to perform checkout runs of this capability at the present time.

### 3. INPUT GUIDE

#### 3.1 BOLTZMANN CODE INPUT INSTRUCTIONS

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
1	1	NCASE – Integer designating number of gas mixtures to be computed ( $NCASE \leq 9$ )	I1
2	1	MIX – Number of gases in first mixture ( $MIX \leq 5$ )	I1
3.1	1-10	LIST(1) – Name of first gas in first mixture (left adjusted)	A10
	11-20	FSI(1) – Parts of first gas in first mixture	F10.0
	21-30	I AVG(1) – Lowest vibrational level of range over which vibrational excitation rate is to averaged (right adjusted)	I10
3.2	1-10	LIST(2) – Name of second gas in first mixture	A10
	11-20	FSI(2) – Parts of second gas in first mixture etc.	

Continue card group 3 for up to 5 gases in the first mixture ( $MIX \leq 5$ ). If  $NCASE > 1$ , i.e., if more than one mixture is to be computed, repeat the sequence for each new gas mixture starting with card 2. Up to 9 mixtures can be computed within one run.

#### 3.2 EDLAMP INPUT INSTRUCTIONS

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
1	1-80	TITLE – Run identification	8A10
2	1-5	MPSI – Initial number of grid points along $\Psi$ coordinate ( $MPSI \geq 3$ )	I5

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
2	6-10	NTYPE - Flow-type option; 0: Axisymmetric flow* 1: Plane flow	15
	11-15	ITURB - Viscosity option; -3: Sutherland laminar + 2 Eq. TKE -2: Sutherland laminar + 1 Eq. TKE -1: Sutherland laminar 0: Constant viscosity	15
	16-20	NS - Number of species (excluding catalytic species)	15
	21-25	NM - Number of catalytic species	15
	26-30	NV - Number of lasing transitions	15
	31-35	NR - Number of reactions	15
	36-40	NT - Number of temperature points in the thermodynamic data tables	15
	41-45	IFROZ - Kinetics option; 0: Reacting flow 1: Frozen flow (omit card groups 20 and 21)	15
	46-50	IPRESS - Pressure or area option; (see Section 2.2) 0: Specified pressure distribution 1: Specified flow area distribution	15
	51-55	ITYPE - Control flag that specifies the form in which the pressure or area data will be input. -1: Pressure or area will be input via a third order polynomial in x (see card 29) 0: Pressure or area will be constant 1: Pressure or area data will be input in tabular form (see card 30)	15
	56-60	KBL - Set to zero. Set to unity if ILOOP > 0.	15
	61-65	NAP - The number of (x, pressure) or (x, area) points to be input in data table when ITYPE = 1 (omit if ITYPE = -1, 0)	15
	66-70	NXTW - Set to zero, unless KBL > 0. See card 31.	15

\* Not applicable for power-on laser cavity calculations or prescribed area calculations.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
2	71-75	JSTEP - Integration step size control; specifies the number of steps for which the integration step size is kept equal to the initial step size. Automatic step size control occurs after JSTEP axial steps.	15
3	1-5	NSKIP - Flowfield data output control parameter; to reduce output frequency, only every NSKIPth station will be printed.	15
	6-10	IOUT1 - Output option for net rate of production 0: No output 1: $\dot{w}$ is output for each species for all lateral points where $T \geq 50K$	15
	11-15	IOUT2 - Output option for forward and backward production rates 0: No output 1: RP and RM are output for each reaction at all lateral points where $R \geq 50K$	15
	16-20	ICON - Output option for species concentrations (mole/cm <sup>3</sup> ) 0: No output 1: Concentrations are output for all species at all lateral points	15
	21-25	KFLAG - Output option for chemical laser information 1: Condensed output (for pulsed calculations) 2: Detailed output for each transition and each grid point	15
	26-30	IPLOT - Control parameter for the printer plot routine 0: Omit printer plots (omit card 28) 1: Printer plots are desired 3: Printer plot of total specific power as a function of axial distance	15
	31-35	NSTART - The first output station for which printer plots are desired.	15
	36-40	NSTA - The number of output stations between printer plots.	15

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
3	41-45	NSPEC - Total number of parameters to be printer plotted (NSPEC $\leq$ 3 + NS). Includes velocity, temperature, density, species mole fraction. Power is not included as a parameter to be plotted.	15
	46-50	IWPWR - Power plot parameter 0: Power plot is not desired. 1: Plot total specific power as a function of axial distance.	15
	51-55	NPWRST - The number of output stations between storage of total specific power and axial distance data. A maximum of 50 data points (power, distance) may be printer plotted.	15
4	1-5	KPWR - Radiation option -1: Flow calculation only (omit cards 22 through 27) 0: Power off 1: Power on	15
	6-10	LFLAG - Line broadening option 0: Doppler broadening only 1: Doppler and Lorentz broadening	15
	11-15	ITL - Direct combustion or transfer laser option 0: Direct combustion laser (HF, DF, AB) 1: Transfer laser (HF-CO <sub>2</sub> , AB-CO <sub>2</sub> )	15
	16-20	IPULS - Laser operations flag 0: CW operation (see Section 2.3) 1: Pulsed operation (see Section 2.2)	15
	21-25	ILOOP - Recirculation loop flag 0: Single pass (open cycle) calculation 1: Multiple pass calculation (closed cycle)	15
	26-30	NPASS - Number of passes through recirculation loop to be computed, less one.	15
	31-35	JRAMP - E-beam current density flag 0: Full E-beam current density 1: E-beam current density will be gradually increased to nominal value over the discharge pulse duration (see Card 9).	15

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
4	36-40	NRCUT - Number of reactions to be retained downstream of electric discharge region. (Note: All reactions beyond NRCUT will then be neglected downstream of discharge and in recirculation loop.)	I5
	41-45	IMP - Chemistry flag 0: Explicit chemistry 1: Implicit chemistry	I5
	46-50	NNEU - Number of neutral species	I5
	51-55	NNEG - Number of negative species, including secondary electrons (but not primary electrons)	I5
	56-60	NPOS - Number of positive species	I5
<b>Note:</b> NNEU, NNEG and NPOS are needed to compute global rates. Species must be input in sequence, first neutrals, then negatively charged particles, then positively charged particles. NNEU + NNEG + NPOS = NS (see Card 2).			
5	1-10	RJ - Reference length; nozzle radius or width (cm) in the y-direction	E10.3
	11-20	XK2 - Viscosity (g/cm-sec) when using ITURB = 0. Omit for ITURB < 0	E10.3
	21-30	XLE(1) - Lewis number (laminar)	E10.3
	31-40	SIGMA(1) - Prandtl number (laminar)	E10.3
6	1-10	X - Initial value of x (cm)	E10.3
	11-20	XMAX - Final value of x (cm)	E10.3
	21-30	PRNT - Output print increment (cm)	E10.3
	31-40	DX - Initial integration step size (cm)	E10.3
	41-50	HALVE - Relative amount to increment DX after JSTEP number of axial steps	E10.3
	51-60	DOUBLE - Maximum allowable integration step size (cm)	E10.3
	61-70	CXD - A constant multiplier that limits integration step size for nonradiating plane flows	E10.3
	71-80	CDX - A constant multiplier that limits integration step size for radiating reacting flows	E10.3
7	1-10	P - Pressure (torr) at initial value of x	E10.3
8.1	1-10	XEB - Location of upstream edge of E-beam window (cm)	E10.3

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
8.1	11-20	EBLEN - Effective length of E-beam window (cm)*	E10.3
	21-30	XDF - Location of upstream edge of discharge electrodes (cm)	E10.3
	31-40	DFLEN - Effective length of discharge electrodes (cm)*	E10.3
	41-50	YDRF - Upstream (x = XDF) discharge electrode separation half-width (cm)	E10.3
	51-60	THETA - Discharge electrode divergence half-angle (rad)	E10.3
8.2	1-10	ACAV - Cavity flow entrance cross-sectional area (cm <sup>2</sup> )	E10.3
	11-20	XCAV - Cavity exit location (cm)*	E10.3
	21-30	XSTART - Presently not used (see Section 2.2)	E10.3
9.1	1-10	EBE - Effective beam electron energy (keV)	E10.3
	11-20	EBJ - Effective post-foil electron beam current density (A/cm <sup>2</sup> )	E10.3
	21-30	VOLTAP - Applied discharge electrode potential (volt)	E10.3
	31-40	CAFALL - Cathode fall potential (volt)	E10.3
9.2	1-10	CVD1 - C <sub>1</sub> , drift velocity curve fit coefficient (see Vol. I, Eq. (16))	E10.3
	11-20	CVD2 - C <sub>2</sub> , drift velocity curve fit coefficient	E10.3
	21-30	CVD3 - n, drift velocity curve fit coefficient	E10.3

Note: Read cards 10.1 through 10.5 only if ILOOP = 1, omit otherwise. On cards 10.2, 10.4 and 10.5, data sequence must correspond to that on card 11. If data on card 10.3 are zero, omit cards 10.4 and 10.5.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
10.1	1-10	DX2 - Integration step size for Region II (see Fig. 1)	8E10.3
	11-20	DX3 - Integration step size for Region III (see Fig. 1)	8E10.3

\*Distance along direction of flow, or corresponding time interval.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
10.2	1-5	CRE(1) - Catalyst removal efficiency for first species	16F5.2
	6-10	CRE(2) - Catalyst removal efficiency for second species, etc.	16F5.2
		Continue for all species observing specified format.	
10.3	1-10	RATE1 - Air leak rate into flow (g/sec)	E10.3
	11-20	RATE2 - Laser gas makeup rate into flow (g/sec)	E10.3
10.4	1-10	RALPH1 (1) - Mole fraction of first species in air leak rate	7E10.3
	11-20	RALPH1 (2) - Mole fraction of second species in air leak rate, etc.	7E10.3
10.5	1-10	RALPH2 (1) - Mole fraction of first species in laser gas makeup rate	7E10.3
	11-20	RALPH2 (2) - Mole fraction of second species in laser gas makeup rate, etc.	7E10.3

Note: For descriptions of cards 11 through 18, assume that there are 13 grid points along the lateral ( $\psi$ ) coordinate.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
11.1.1	1-10	Mole fraction of first species at first $\psi$ point, $y = 0$	7E10.3
	⋮		
	61-70	Mole fraction of seventh species at first $\psi$ point, $y = 0$	7E10.3
11.1.2	1-10	Mole fraction of eighth species at first $\psi$ point, $y = 0^*$	7E10.3
11.2.1	1-10	Mole fraction of first species at next grid point	7E10.3
	⋮		
	61-70	Mole fraction of seventh species at next grid point	7E10.3
11.2.2	1-10	Mole fraction of eighth species at next grid point	7E10.3

\* For illustration purposes, it is assumed that there are eight species in a given problem. Lasing species are given first, in order  $v = 0, v = 1, v = 2$ , etc.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
11.13.1	1-10	Mole fraction of first species at 13th grid point	7E10.3
	⋮		
	61-70	Mole fraction of seventh species at 13th grid point	7E10.3
11.13.2	1-10	Mole fraction of eighth species at 13th grid point	7E10.3
12.1	1-10	U(1), Velocity (m/sec) of first $\Psi$ point, $y = 0$	7E10.3
	⋮		
	61-70	U(7)	7E10.3
12.2	1-10	U(8)	7E10.3
	⋮		
	51-60	U(13), Velocity (m/sec) of last $\Psi$ point	7E10.3
13.1	1-10	T(1), Temperature (K) of first $\Psi$ point, $y = 0$	7E10.3
	⋮		
	61-70	T(7)	7E10.3
13.2	1-10	T(8)	7E10.3
	⋮		
	51-60	T(13), Temperature (K) of last $\Psi$ point	7E10.3
14.1	1-10	Y(1), y coordinate (cm) of first $\Psi$ point	7E10.3
	11-20	Y(2), y coordinate (cm) of second $\Psi$ point	7E10.3
	⋮		
	61-70	Y(7), y coordinate (cm) of seventh $\Psi$ point	7E10.3
14.2	1-10	Y(8), y coordinate (cm) of eighth $\Psi$ point, etc.	7E10.3

NOTE: The following four card groups (15, 16, 17 and 18) contain input for the turbulence models (ITURB = -2, -3). Omit these cards if ITURB  $\neq$  -2, -3.

15.1	1-10	UP(1), Relative fluctuating component of velocity of first $\psi$ point, $y = 0^*$	7E10.3
	⋮		

\*Typical values for UP, TP and AP are on the order of 0.01.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
15.1	51-60	UP(7)	7E10.3
15.2	1-10	UP(8)	7E10.3
	⋮		
	51-60	UP(13), Relative fluctuating component of velocity of last $\psi$ point	7E10.3
16.1	1-10	TP(1), Relative fluctuating component of temperature of first $\psi$ point, $y = 0$	7E10.3
	⋮		
	61-70	TP(7)	7E10.3
16.2	1-10	TP(8)	7E10.3
	⋮		
	51-60	TP(13), Relative fluctuating component of temperature of last $\psi$ point.	7E10.3
17.1	1-10	AP(1, 1), Relative species fluctuating component of first $\psi$ point, $y = 0$	7E10.3
	⋮		
	61-70	AP(1, 7)	7E10.3
17.2	1-10	AP(1, 8)	7E10.3
	⋮		
	51-60	AP(1, 13), Relative species fluctuating component of last $\psi$ point	7E10.3
18.1	1-10	SL(1), Scale of turbulence (cm)	7E10.3
	⋮		
	61-70	SL(7)	7E10.3
18.2	1-10	SL(8), etc.	7E10.3

NOTE: Card 18 is read only if ITURB = -3, and is omitted otherwise.

The following cards contain the thermodynamic data. The order of the species must be identical to the order on cards 10 or 11. Lasing species data must be given first, in the order  $v = 0$ ,  $v = 1$ ,  $v = 2$ , etc. The first card contains the species name, molecular weight and heat of formation. The second and

remaining cards contain the temperature and corresponding specific heat, entropy and enthalpy for that species. Two temperatures and corresponding thermodynamic data are placed on each card. The data are input exactly as presented in the JANAF tables with the temperature points being the same for all species. Number of temperature points must be specified at NT (see card 2).

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
19.1.1	1-6	Name of first species	A6
	7-16	Molecular weight	E10.3
	17-26	Heat of formation, $h_{298_i}$ (kcal/mole)	E10.3
19.1.2	1-10	First temperature point (K)	F10.4
	11-20	$c_{p_i}$ (cal/mole-K)	F10.4
	21-30	$S_i$ (cal/mole-K)	F10.4
	31-40	$h_i - h_{298_i}$ (kcal/mole)	F10.4
	41-50	Second temperature point (K)	F10.4
	51-60	$c_{p_i}$ (cal/mole-K)	F10.4
	61-70	$S_i$ (cal/mole-K)	F10.4
	71-80	$h_i - h_{298_i}$ (kcal/mole)	F10.4
19.1.3	1-10	Third temperature point	F10.3
		⋮	
		⋮, etc.	

NOTE: The following set of cards specifies the catalytic species (M1, M2, M3, ...) and their respective composition in terms of the species participating in the reactions. Weighting factors must be read in the same order in which the thermodynamic data sets are read. Omit card group 20 if IFROZ = 1.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
20.1.1	1-6	AID(NS+1) - Name of first catalytic species (e.g., M1)	A6
20.1.2	1-5	WF(1, 1) - Weighting factor of first species (for first catalytic species). Set weighting factor to zero for any reactant which does not contribute to the respective catalytic species.	16F5.2

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
20.1.2	6-10 : :	WF(1, 2) – Weighting factor of second species contributing to first catalytic species	16F5.2
	75-80	WF(1, 16) – Weighting factor of 16th species contributing to first catalytic species	16F5.2
20.1.3	1-5	WF(1, 17) – Weighting factor of 17th species contributing to first catalytic species, etc.	16F5.2
20.2.1	1-6	AID(NS+2) – Name of second catalytic species	A6
20.2.2	1-5	WF(2, 1) – Weighting factor of first species contributing to second catalytic species, etc.	16F5.2
20.NM.1	1-6	AID(NS+NM) – Name of last catalytic species, etc.	A6

The following set of cards specifies the chemical reaction mechanisms for a particular problem, one card for each reaction. No particular order is required. Omit card group 21 if IFROZ = 1. Also see NRCUT (card 4).

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
21.1	1-6	Species A	A6
	7	+ sign	A6
	8-13	Species B (or M)	A6
	14	+ sign	A6
	15-20	Blank (or M)	6x(A6)
	21	= sign	A6
	22-27	Species C	A6
	28	+ sign (if needed)	A6
	29-34	Species D (or M)	A6
	35	+ sign (if needed)	A6
	36-41	Species E (or M)	A6
	43	Global rate indicator	I1
		1: Primary ionization	
		2: Secondary ionization	
		3: Electron-ion recombination	
		4: Ion-ion recombination	
		5: Electron attachment	
		6: Electron detachment	

This indicator is omitted for any reaction not falling into one of the above categories.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
21.1	42-48	Blank	7x
	49-50	Reaction type, 1 to 15	I2
	51	Rate constant type 1 to 10 (Read 0 for type 10)	I1
	52-59	A, pre-exponential factor (cm-particle-sec units)	E8.2
	60-64	N, temperature exponent	F5.2
	65-74	B, activation energy (cal/mole)	E10.3
	75-80	M, temperature exponent	F6.2

NOTE: If the rate constant type is either 7 or 8, a second card must be used to read values for  $A_1$ ,  $N_1$ , and  $B_1$ .

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
21.1.1	52-59	$A_1$ , pre-exponential factor	E8.2
	60-64	$N_1$ , exponent	F5.2
	65-74	$B_1$ , exponential factor	E10.3
21.2		Next reaction	
21.NR		Last reaction	

The following cards specify the necessary input for laser calculations. Omit cards 22 through 27 if KPWR = -1.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
22	1-10	WLM - Molecular weight of the lasing species	E10.3
	11-20	System constants $\omega_e$ , $\omega_e x_e$ , $B_e$ and $\alpha_e$ (1/cm) of the lasing molecule	E10.3
	21-30		
	31-40		
	41-50		
	51-60	RAS - Resonance broadening constant $a^*$ ( $K^{1/2}/\text{cm-atm}$ )	E10.3
	61-70	RBS - Resonance broadening constant $b^*$ ( $K/\text{cm-atm}$ )	E10.3

NOTE: The following card group specifies the collision broadening constants,  $a_j$  ( $j=1, NS$ ), one for each species, in the same order in which the thermodynamic data sets are read.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
23.1	1-10 : : 71-80	RA(1) - Collision broadening constant for first species  RA(8) - Collision broadening constant for eighth species	8E10.3  8E10.3
23.2	1-10	RA(9) - Collision broadening constant for ninth species, etc.	8E10.3
24	1-10 11-20 21-30 31-40 41-50	AB } BB } Curve-fit coefficients for the matrix CB } elements of the dipole moment for the AV } v = 1 — v = 0 transition of the lasing BV } molecule	E10.3

Card 25 contains information to evaluate the cavity threshold gain level for a Fabry-Perot cavity. Using appropriate mirror reflectivities, this value will indicate the level of the loaded gain.

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
25	1-10   11-20   21-30   31-40   41-50 51-60 61-70 71-80	R1 R2 } Cavity mirror reflectivities  AC1 AC2 } Cavity mirror loss coefficients  CL - Active medium width (cm) Not used AW1   AW2   Window loss coefficients	E10.3  E10.3  E10.3 E10.3  E10.3
26	1-5 6-10	JFIX(1)   Lower level rotational quantum JFIX(2)   numbers for all transitions (1, NV) for operation at fixed J	1615
If JFIX(1) values are input as zero, the program will locally select all J-values based on the highest gain (J-shifting).			
27	1-80	ISET(1) - Lasing option; a value (0 or 1) must be input for NV number of lasing transitions  ISET(1) = 0: No lasing : 1: Lasing :  ISET(NV) = etc.	1615

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
28	1-80	IPLTYP(1) - Input control array for parameters to be printer plotted ( $1 \leq 3+NS$ ) IPLTYP(1) = 1: Velocity 2: Temperature 3: Density xx4: Species mole fraction (where xx refers to a particular species, i.e., $1 \leq xx \leq NS$ )	1615

NOTE: The control flags for the parameters to be printer-plotted may be input in any order as long as a 1615 format is followed. The species control flag (xx) refers to a particular species to be plotted. Each species is numbered corresponding to the order in which that species was input in thermodynamic data. Omit card 28 if IPLOT = NSPEC = 0. Cards 29 and 30 concern the specification of a streamwise pressure (IPRESS = 0) or cross-sectional area (IPRESS = 1) distribution either by a third order polynomial (ITYPE = -1), or by tabular input (ITYPE = 1).

$$ITYPE = \begin{cases} -1: & \text{read 29, omit 30} \\ 0: & \text{omit 29, 30} \\ 1: & \text{omit 29, read 30} \end{cases}$$

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
29	1-10	APC(1) - Pressure coefficient (torr) Area coefficient ( $\text{cm}^2$ )	E10.3
	11-20	APC(2) - Pressure coefficient (torr/cm) Area coefficient (cm)	E10.3
	21-30	APC(3) - Pressure coefficient ( $\text{torr}/\text{cm}^2$ ) Area coefficient (cm)	E10.3
	31-40	APC(4) - Pressure coefficient ( $\text{torr}/\text{cm}^3$ ) Area coefficient (1/cm)	E10.3

NOTE: The pressure (or area) coefficients are used in the following polynomial expression:

$$P(X) = APC(1) + APC(2)X + APC(3)X^2 + APC(4)X^3$$

<u>Card</u>	<u>Col.</u>	<u>Description</u>	<u>Format</u>
30.1	1-80	APX(I), APV(I) - Pressure or area table (I = 1, 4), i.e., four (x, pressure) or (x, y) points are input per card. The NAP parameter (card 4), gives the total number of data points to be input. If IPRESS = 0; x (cm), Pressure (torr) If IPRESS = 1; x (cm), y (cm)	8E10.3
30.2	1-80	APX(I), APV(I), I = 5, 8	8E10.3
30.3	1-80	APX(I), APV(I), I = 9, 12, etc.	8E10.3

NOTE: If KBL = 0 (card 2), omit card group 31. If ILOOP = 1 (card 4), card group 31 is used to specify the laser gas temperature in the recirculation loop, Region III.

31.1	1-80	XTW(I), TW(I) - Wall temperature table (I = 1, 4), i.e., four (x, $T_{wall}$ ) points are input per card. The NXTW parameter, (card 2), gives the total number of data points to be input. (x(cm); $T_{wall}$ (K)).	8E10.3
31.2	1-80	XTW(I), TW(I), I = 5, 8	8E10.3
31.3	1-80	XTW(I), TW(I), I = 9, 12, etc.	8E10.3

NOTE: The following (and last) card concerns the grid point control scheme which is explained in Section 3.3.2 (not applicable for EDL).

32	1-5	IDS - grid point control flag	15
		0: No grid points will be eliminated	
		1: Grid points will be eliminated if possible	15
	6-10	IDROP - Maximum number of grid points to be dropped	15
	11-20	DELUP - Control parameter (see Section 3.2.2)	E10.3
	21-30	DELUP1 - Control parameter (see Section 3.2.2)	E10.3

### 3.3 HINTS FOR PROGRAM OPERATION

#### 3.3.1 Prescribed Cross-Sectional Area

This option allows input of a flow cross-sectional area distribution via cards 29 or 30, thereby "indirectly" specifying the pressure distribution

to be used in solving the boundary layer conservation equations. For combustion lasers, experimental evidence appears to indicate that most cavity flows are closer to constant cross-sectional area flows than to constant pressure flows (usually accompanied by rather strong expansions due to the thermal energy release in the combustion).

### 3.3.2 Streamline Control Scheme

Calculations with boundary layer profiles require a relatively fine lateral gridpoint spacing initially which causes the axial step size to remain unnecessarily small as the velocity profile becomes more uniform farther downstream from the initial station. The purpose of the streamline control scheme is to shorten run times by dropping out lateral grid points as they become unnecessary, thus eliminating small  $\Delta\psi$ , and consequently permitting a larger axial step size to be used. Computer run times for cases with streamline control have been reduced from 1/2 to 1/10 of the unmodified case run time.

Use of this scheme is controlled via the card 32 containing four parameters: IDS, IDROP, DELUP, DELUP1 (format 2I5, 2E10.3). A blank card must be inserted if no streamlines are to be dropped.

A value of IDS = 1 indicates that grid points are to be dropped. IDROP specifies the maximum but not necessarily the total number of grid points to be dropped. DELUP and DELUP1 are control criteria which must be satisfied concurrently before a grid point is dropped. Their function is best described as follows. The use of velocity boundary layer profiles as initial values initially sets the difference between the minimum and the maximum velocity in the flow field to be computed. As the two adjacent boundary layers mix, diffusion will generally cause a reduction in this difference between the minimum and the maximum velocity. The first streamline control criterion is satisfied when the current difference between the maximum and minimum velocity in the flow field has reached a certain fraction of the initial difference.

This value is set by DELUP and from experience ranges from 0.5 to 0.8. Thus, the smaller DELUP, the farther downstream will this criterion be satisfied. Once this test is satisfied the flow field is searched to determine the grid points adjacent to the minimum  $\Delta\psi$ . A check is made to deduce the effect on the velocity profile of eliminating either one of the two grid points adjacent to the  $\Delta\psi$ . The smaller of the two effects is compared to a prescribed tolerance (DELUPI) and if satisfied allows a grid point to be dropped. From experience, DELUPI ranges from 0.2 to 0.5. Successive grid points are dropped in a similar manner as the velocity profile becomes more uniform.

### 3.3.3 Internal Program Messages and Diagnostics

- "TEMPERATURE OUT OF RANGE." The temperature for a particular species is outside the temperature range of the input thermodynamic data. This is not necessarily an error message. Check the input data. If no errors are found and the temperature seems unusual (i.e., a negative temperature) reduce the step size by altering the appropriate multiplier.
- "NORMAL TERMINATION - X = XMAX." The program has terminated because the axial program limit (XMAX) has been reached.
- "NEGATIVE MOLE FRACTION ENCOUNTERED." When this error message is encountered, check the input data. If no errors are found, reduce the integration step size by modifying the appropriate multiplier.
- "X OUT OF RANGE - \*\*\*\*\* DATA TABLE." The program has terminated because the current value of x exceeds the maximum value of x input in the \*\*\*\* (pressure, area, wall temperature) data table.

### 3.3.4 Plot Routines and Flowfield Tape Generation

As part of the output option included in the EDLAMP code, the program user may, by specifying input control flags, obtain on-line printer plots of pertinent variables.

- The lateral distribution of the local values of temperature, molecular weight, density, velocity and chemical species mass or mole fractions at specific axial stations within the flow field.

- Integrated averages of the quantities listed above as a function of axial distance through the flow field.
- Total specific power as a function of axial distance.

The printer plot routine is controlled by the following input parameters: IPLOT, NSTART, NSTA, NSPEC, IWPWR, NPWRST and the IPLTYP array. The following is a description of the input parameters.

<u>Input Parameter</u>	<u>Description</u>
IPLOT	The input control flag which specifies whether or not data are to be output via printer plots. IPLOT = 0, omit printer plot routines. IPLOT = 1, produce printer plots of the parameters specified by the IPLTYP array and the IWPWR control flag. IPLOT = 3, produce printer plot of total specific power versus axial distance at the last axial station.
NSTART	The output station at which the first printer plots are to be produced.
NSTA	The number of output stations between printer plots. On-line printer plots begin initially at NSTART and every NSTA stations thereafter.
NSPEC	Total number of parameters to be printer plotted (3+NS max). Parameters include: velocity, temperature, density and species mole fraction. Power is not included in NSPEC as a parameter to be plotted.
IWPWR	Power plot control flag. IWPWR = 0, omit printer plot of power versus axial distance. IWPWR = 1, printer plot of total specific power versus axial distance at last axial station is desired.
NPWRST	This parameter is used only when IWPWR = 1. The number of output stations between storage of power data. The program will handle a maximum of 50 data points (total specific power, axial distance).
IPLTYP	This array specifies which parameters are to be printer plotted. There will be NSPEC values input in the following manner: <ul style="list-style-type: none"> <li>1: Velocity</li> <li>2: Temperature</li> <li>3: Density</li> <li>xx4: Species mole fraction of the xx<sup>th</sup> species</li> </ul> The control flags for the parameters to be plotted may be input in any order as long as a 1615 format is followed.

Printer plots will be output in the same order as found on the data card. The species mole fraction control flag (xx) designates a particular species mole fraction to be plotted. Each species is numbered corresponding to the order in which that species was input in the thermodynamic data.

The input parameters discussed above are read on card 3, except IPLTYP which is read on card 28.

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