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The Possibility of Hot Reaction Enhancement of CW HF Laser Performance

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Continuous wave (cw) lasing on the vibrational levels pumped by the HF hot reaction have been successful in the past, but total powers were less when operating on the H_2-F_2 chain reaction than when operating on the HF cold reaction. Optimal conditions for the H_2-F_2 chain reaction were reported at a fluorine dissociation fraction of approximately 0.03 to 0.05. Because the computational models employed in these early studies did not include the collisional decomposition of HF(v ≥ 3) by H atoms, these models overpredicted performance by a factor of 15 to 30. When these reactions were included in the computer model, the predictions were within a factor of 2 to 6 of the experimental data. Computer simulation of both arc and combustion driven cw HF lasers showed that four conditions are necessary to obtain increased laser performance from the HF hot reaction: (1) Reduced fluorine dissociation at the primary nozzle exit plane; (2) The correct total temperature of the primary flow; (3) Proper design of the laser cavity flow channel geometry; (4) The medium must be well saturated. All four of these conditions must be optimized together to obtain increased laser performance from the hot reaction. Satisfying one or two of these by themselves is not sufficient.

I. Introduction

The reaction of H_2 and F_2 to form excited HF takes place in two steps: the "cold reaction":

$$F + H_2 \rightarrow HF(v \leq 3) + H \qquad -\Delta H = 31.5 \text{ kcal/mol} \qquad (1)$$

and the "hot reaction":

$$F_2 + H \rightarrow HF(3 \leq v \leq 6) + F \qquad -\Delta H = 98.0 \text{ kcal/mol} \qquad (2)$$

Since the hot reaction releases more energy and populates higher vibrational bands of HF than the cold reaction, there has been considerable interest in utilization of the hot reaction to increase laser power.

The goals of this study were to determine if it is possible to obtain additional power from cw HF lasers by utilizing the hot reaction and, if so, under what conditions this additional power could be obtained.

Attempts were made by TRW[1,2], UARL[3], and Gastaud et al[4] to obtain increased cw HF laser power from the hot reaction. These studies showed that reducing the fluorine dissociation ratio in the primary stream to approximately 0.03 to 0.05 generated a hot/cold chain reaction. Unfortunately, the total power output was lower than expected. Simulation of the experiments performed by TRW[1], UARL[3], and Bell Aerospace Textron[5] predicted 15 to 30 times more power than was observed. These models did not include the collisional decomposition of HF(v ≥ 3) by H atoms. A brief review of these prior attempts to utilize the hot reaction in cw HF lasers is presented in Section II. The mathematical modeling predictions, experimental data, and major conclusions of these studies are summarized.

When the TRW cw HF hot reaction experiment was modeled with the rotational equilibrium BLAZE II[6] code with the kinetics set containing the collisional decomposition of HF(v ≥ 3) by H atoms, the predicted power was within a factor of two of the data. The CL-XI combustion-driven cw HF laser[7] was modeled with changes made to operate on the hot reaction. These simulations showed that additional power could be obtained from a combustion

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driven cw HF laser utilizing the hot reaction. The results of these modeling studies are presented in Section III and concluding remarks are given in Section IV.

II. Review of CW HF Chain and Hot Reaction Chemical Laser Studies

In the following sections, the studies of TRW, UARL and Gastaud are reviewed to provide a point of departure for this study.

2.1 TRW HF Chain Reaction Laser Experiments

TRW conducted several sets of experiments studying lasing on the HF hot reaction. One set of experiments employed an arc-driven cw HF laser with their HCl-II nozzle[1]. The fluorine dissociation fraction was varied by changing arc power. Closed cavity power measurements were made using gold-coated mirrors. The power was measured calorimetrically. With no mirrors on the laser, chemiluminescence measurements were made of HF(v) number density and rotational temperature.

2.1.1 Model

In order to initiate the chain reaction, it is necessary to have both undissociated F_2 molecules and dissociated F atoms in the flow. The ratio of F_2 molecules to F atoms in the flow is represented by the dissociation fraction "alpha" (α), defined as:

$$\alpha = \frac{\dot{m}(F)}{\dot{m}(F) + \dot{m}(F_2)} \tag{3}$$

where $\dot{m}$ is the mass flow per unit time of the species in parenthesis. TRW obtained dissociated fluorine by using an electric arc to heat F_2 and diluent.

TRW conducted a parametric analysis using the RESALE-3 code to determine the optimum flow conditions for extracting laser power from the chain reaction. The RESALE-3 code used Cohen's 1972 HF rates[8], with the addition of HF(v) deactivation by DF and CF_4 [1]. The predicted performance as a function of α is shown in Table 1.

Table 1. TRW RESALE-3 prediction of performance as a function of α.[1]

α	Total mass flow rate (g/sec)	Power (kW)	Specific Power (kJ/g)	Specific Power (kJ/g F)	Lasing cutoff (cm downstream)
0.05	64.8	75.3	1.16	2.70	44.8
0.1	64.5	73.5	1.14	2.64	24.6
0.2	63.9	62.4	0.98	2.26	16.0
1	59.7	13.4	0.22	0.52	9.2

There is little change in power or specific power between the $\alpha = 0.05$ and the $\alpha = 0.1$ cases, but at $\alpha = 0.05$, the cutoff distance is almost twice that at $\alpha = 0.1$. Best power is obtained at $\alpha = 0.05$, where F_2 is abundant and the hot reaction is presumably contributing. The findings of the parametric study are summarized as follows:

1. Total power output was predicted to increase with decreasing alpha.
2. Maximum power was obtained at $\alpha = 0.05$, where power was a factor of 5.6 greater than for the fully dissociated case.
3. Lasing cutoff increased as α decreased, becoming a factor of 4.8 greater than the fully dissociated case when $\alpha = 0.05$.

The results of this modeling study suggested that to obtain chain operation, the laser should be run with small $\alpha = 0.05$.

2.1.2 Experiments

The experiments by TRW[1] were performed using an arc-driven cw HF laser. A 1/2" x 7", 5-to-1 expansion area ratio nozzle (HCl-II) with 72 fluorine nozzles with 1/2" x 0.010" throat dimensions and 71 1/2" x 0.002" hydrogen slits was used. Gold coated 98% reflective mirrors (10 cm x 10 cm) were used to measure closed cavity power. The baseline flow rates of the gases were: F_2 = 2 g/sec, Argon = 40 g/sec, and H_2 = 1 gm/sec. A factor of two to three excursion was made in each of these flow rates. A cavity pressure of 9 torr was chosen for the baseline case, with excursions from 5 to 30 torr. Arc power was varied from 5 kw to 47 kw; at 5 kw, the fluorine dissociation fraction (α) was about 0.03 and at 47 kw about 1.0. Minimum laser power was observed at an arc power of 6 kw, with greater laser power at 5 kw. Because of this, TRW believed their laser to be fully operating on the chain at 5 kw arc power, for which $\alpha = 0.03$.

The increase in laser power when arc power was decreased from 6 kw to 5 kw was described as "encouraging" by TRW[1]. The total laser power at 5 kw arc power was about 100 watts, a factor of 30 below the RESALE-3 predictions. Since power was observed from the $v = 5 \rightarrow 4$ and $v = 4 \rightarrow 3$ bands, which are pumped by the hot reaction, chain reaction lasing was achieved. The predicted distribution of power from different vibrational bands was similar to the measured powers. RESALE-3 predicted power on the $7 \rightarrow 6$ and $6 \rightarrow 5$ bands while, experimentally, no power was observed on these bands. Although lasing on the upper vibrational bands was achieved, clearly indicating successful chain reaction, the total power output was much lower than anticipated.

2.2 TRW HF Hot Reaction Studies

After the first set of experiments on chain reaction lasing, TRW launched an experimental and theoretical investigation into the basic mechanisms of the chemical mixing reaction process.[2] Part of the study involved an analytical look at hot reaction lasing, and tested several different methods for initiating the HF hot reaction. These experiments were conducted in their Reactive Flow Test Facility. This facility used the RF-2 nozzle, which consisted of two parallel supersonic nozzles fed by separate supply systems. Both supply systems had their own primary, secondary, and/or arc jet heater system, depending on the requirements of the experiment.

The hot reaction was studied in 16 tests by running undissociated fluorine and diluent through one nozzle and dissociated hydrogen and diluent through the other. Two different methods were used to dissociate the hydrogen: 1) by bulk gas-gas heat transfer of arc-jet heated nitrogen, and 2) by passing molecular hydrogen directly through the arc-jet head with the diluent. The tests included spectral emission measurements, absorption/gain measurements, and infrared mapping of chemiluminescent HF and DF emission in the 2.4 to 4.4 micron region to obtain a full 2-D picture of the flow field. The objective of these measurements was to examine the kinetic rate coefficients used in TRW's analytical models, particularly those associated with the upper vibrational levels pumped by the hot reaction. Comparison with predictions from the Blottner code[9] allowed TRW to formulate a new set of rate coefficients in conjunction with N. Cohen of the Aerospace Corporation. The principal difference between these new rates and the 1972 rates was the inclusion of multi-quantum HF(v) transitions. Using these new rates with the Blottner code resulted in a decrease in the extent to which the model overpredicted the HF(v) concentrations for $v \geq 3$. Unfortunately, the model still overpredicted. At this stage in the investigation, it became clear that accurate measurements of the hydrogen dissociation could not be achieved, and the hot reaction experiments were halted.

The H_2-F_2 chain reaction was studied in five tests using both nitrogen and argon diluents. The chain was initiated by heating F_2 and diluent in one jet using an electric arc; fluorine plenum temperatures were varied from 500K to 1700K. The other jet contained H_2 and diluent. Measurements were made of the flow field and compared to the Blottner code predictions. The new rates were found to improve the agreement between theory and experiment for the chain reaction, but the predicted populations of the upper vibrational bands of HF were still much higher than the measurements.

For the thermally initiated chain reaction, TRW concluded that:

1. The pumping rates for both the cold and hot reactions in the Cohen 1972 rate package are approximately correct.
2. There is an error in the chemical rates associated with the deactivation of the high vibrational levels pumped by the hot reaction.
3. The inclusion of multi-quantum HF(v) transitions that redistribute the vibrational energy in favor of the HF(0) and HF(1) greatly improves the agreement between theory and experiment. However, the theoretical predictions of excited state distributions was still too optimistic.

TRW does not report any power predictions with the modified rates. The TRW power extraction experiments[1] suggest that to obtain chain reaction lasing, α should be small, on the order of 0.03 to 0.05.

2.3 UARL HF Hot Reaction Studies

Experiments done at UARL[3] and summarized by Bell Aerospace Textron[5] appear to be similar to TRW's arc-driven experiments[1]. Since the original UARL reports are not available, the information about these experiments was obtained from Ref. 5. The limited details in the Bell report indicate that UARL used a mass heater to thermally dissociate fluorine and initiate the chain reaction in a cw HF laser device. UARL reported their highest measured power on the chain reaction occurred for an α of 0.05. This supports the results of the TRW experiments, which suggested that $\alpha = 0.03$ was ideal for the chain reaction. UARL demonstrated lasing on vibrational levels $v = 1 - 5$, clearly indicating power from the vibrational levels pumped by the hot reaction. Cavity pressure was as high as 33 torr, substantially higher than TRW's nominal cavity pressure of 9 torr. The UARL experiments ran into significant problems with excessive heat release and thermal choking in the flow. To try to explain the difference between theory and experiment, UARL examined the effect of HF(0) on laser performance. They found that recirculation and entrainment of ground state HF in the laser cavity reduced gains by up to a factor of four. Thus, they concluded that recirculation in the flow channel might be contributing to the differences between the modeling predictions and experiments.

2.4 Gastaud *et al.* HF Hot Reaction Studies

Gastaud et al[4] studied the chain reaction at the Centre de Recherches de la C.G.E. in Marcoussis, France. There is no published modeling of their experiment. Their experimental apparatus used a mass-heater to thermally dissociate a fraction of the F_2. A mixture of partially dissociated fluorine and helium flowed through the primary nozzle. The nozzle consisted of 40 Mach 2.8 primary nozzles alternating with 41 H_2 fuel slits. The stable optical resonator consisted of 5 cm diameter dielectric mirrors. The optical axis could be translated between 0.4 and 3.7 cm downstream from the nozzle exit plane. Two flow channels were employed. Mirrors of different outcoupling fractions were tested, and peak power was obtained at an outcoupling fraction of about 5%. With a 2% outcoupling optical resonator, power was produced from the $v = 5 \rightarrow 4$ and $v = 4 \rightarrow 3$ transitions, which verifies the presence of the HF hot reaction. At this level of outcoupling, 2% of the total power was coming from the $v = 5 \rightarrow 4$ and $v = 4 \rightarrow 3$ transitions. The corresponding α and total power were not given. Apparently, lasing on the upper vibrational bands was observed only with a small outcoupling resonator.

2.5 Summary of Previous Studies

The preceding studies provide several key results. They suggest that the best chain reaction laser performance occurs using a fluorine dissociation ratio (α) of about 0.03 to 0.05. Small outcoupling was necessary to obtain power from the upper vibrational bands, which also suggests low gain on these lines. The hot reaction is accompanied by high levels of heat release and potential problems with thermal choking. Previous analytical models overpredicted the power of lasers operating on the HF hot reaction. The fact that these analytical models did not include the collisional decomposition reactions for HF($v \geq 3$) may be the reason they overpredicted the performance of hot reaction lasers. This possibility will be examined in the next section.

III. Simulation of the HF Hot Reaction Laser

3.1 Introduction

At the time the previous hot reaction and chain laser studies[1-5] were performed, the collisional decomposition of HF(v), $v \geq 3$ by H atoms was not included in any of the computer models of the HF laser. During the development of the efficient, rotational nonequilibrium model of a cw HF chemical laser[10], it was noted that all the very detailed, finite rate, mixing, chemical laser models such as BLAZE II[6], LAMP[11], etc., predict lasing on the upper vibrational bands, $3 \rightarrow 2$, $4 \rightarrow 3$, $5 \rightarrow 4$, $6 \rightarrow 5$, for cases in which these bands are not observed experimentally. It was suggested that the collisional decomposition reaction[12]

$$H + HF(v) \rightarrow H_2 + F \qquad v \geq 3 \qquad (4)$$

is fast enough to significantly reduce the power predicted in the upper vibrational bands. In an experiment which combined chemiluminescence and mass spectrometer measurements, Bartoszek, Manos and Polanyi[13] measured the relative rates for the reactions

$$HF(v) + D \xrightarrow{k^{v}_{CD}} HD + F \qquad (5)$$

$$HF(v) + D \xrightarrow{k^{v,v'}_{ex}} H + DF(v') \qquad (6)$$

for v = 1 to 6. Their data showed that the abstraction reaction (5) is the preferred path until v = 5. At v = 5, the exchange reaction (6) becomes possible. From their plot of the relative rate constant for reactions (5) and (6) versus v, it was concluded that no appreciable formation of DF occurred until v = 6 and that the rate constants for $v \leq 5$ were due to reaction (5) only. The data showed no reaction for v = 1 and 2 with a linear increase in the rate constants for v = 3 to 5 and a large increase in the rate for v = 6. Since the rate for v = 6 was the combined rate for both reaction channels, the rate for reaction (5) for v = 6 was estimated by extrapolating the straight line through the v = 3 to 5 data points to v = 6. The difference between this extrapolated value and the measured rate constant at v = 6 was taken as the rate constant for reaction (6). The experiment of Bartoszek, et al did not determine the vibrational level of DF formed in reaction (6). Following the suggestion of J.C. Polanyi[14], the energy available to populate the various vibrational levels of the product molecule was taken as one half the activation barrier of reaction (6) (49 kcal/mole) plus the difference between the vibrational energy of HF(6) minus the activation barrier energy of reaction (6). Since the resulting energy is sufficient to populate up to HF(3), the product HF(v') was distributed over v' = 1, 2 and 3 in proportion to the ratio $E_{v',v'-1}/ E_{30}$. The relative rates for reactions (5) and (6) as a function of v are given in Table 2, where

$$k^3_{CD} = 2.62E14\ T^{0.179} \exp(-0.76 / RT) \tag{7}$$

Table 2. Rate constants for the abstraction and exchange reactions (5) and (6) as a function of v. k^3_{CD} is in cc/mole sec, T in Kelvins and R in Kcal/mole°K.

v	k^v_{CD} / k^3_{CD}	v'	$k_{ex}^{v,v'} / k^3_{CD}$
3	1		0
4	1.523		0
5	2.237		0
6	2.759	1	0.5344
		2	0.5038
		3	0.4885

The absolute value of the rate constant for reaction (4) for v = 3 was estimated from the data of Bott and Heidner[15]. Since they could not distinguish which reaction channel was occurring in their experiment, Bott and Heidner estimated that 7% of the total reaction rate for the removal of HF(3) was due to reaction (4). Using that estimate as a lower bound and their total removal rate of HF(3) as an upper bound, a series of calculations[10] were performed using BLAZE II to determine a value for the rate constant of (4) for v = 3 (the rates for v = 4, 5, 6 were obtained from Bartoszek's[13] relative rate data), which would result in decreasing the power in the upper bands to values which are below the threshold of the power spectral measurements. The CL-XI experiments[7] provided the power spectral data. It was found that to reduce the power in the upper vibrational bands below the threshold detectable in the power spectral experiments, the rate constant for reaction (5) (the D atom was replaced by an H atom) should be the total removal rate for HF(3) measured by Bott and Heidner[15]. This value, k^3_{CD}, is given in Eq. (7) as a function of T. With this expression for k^3_{CD} and treating the collisional decomposition reactions as one way reactions, the inclusion of reaction (4) effectively eliminated the occurrence of lasing on upper vibrational bands[10].

To determine if this mechanism is responsible for the overprediction of chain laser performance, the BLAZE II rotational equilibrium, quasi-2-D mixing, chemical kinetic, Fabry-Perot laser model including the collisional decomposition of the upper vibrational levels of HF was used to simulate the previous experiments. Since BLAZE II is a rotational equilibrium model, it can predict total power in a given vibrational band, but it cannot predict the spectra in a given vibrational band. The HF kinetics model and rate constants used in the BLAZE II code are given in Ref. 16.

3.2 Modeling the TRW Experiments

Since some of the input data for the TRW experiment were not reported, the missing parameters were estimated based on other data available and on data from Bell Aerospace Textron[5] in their report on modeling TRW's experiments. The static temperatures at the exit of the primary and secondary nozzle flows were taken from the analysis by Bell Aerospace Textron[5]. The areas of the primary and secondary nozzles at the nozzle exit plane were estimated from details of the nozzle bank. TRW reported that the HCl-II nozzle had 72 primary nozzles with 0.5" by 0.010" throat dimensions and a 5 to 1 expansion ratio. For the present study,[16] it was assumed that the 5 to 1 expansion ratio referred to the gas expansion ratio, with the effects of boundary layers included. Thus, the geometric expansion ratio of the primary nozzle could be much greater. With this assumption, the 71 secondary nozzles would take up 0.071 in^2 or 0.458 cm^2. Subtraction of this area from the total nozzle bank area gives 22.12 cm^2 for the primary nozzles. This results in a primary nozzle exit dimension of 0.5" by 0.09525" per nozzle. This implies a geometric expansion ratio of 9.5 (nozzle exit to throat area ratio). The mach number in the secondary slits would be unity, because of the constant area. The primary nozzle mach number was derived from the isentropic area equation. Assuming a 5 to 1 effective area ratio gives an exit Mach number of about 3.2.

It was not reported what kind of resonator was used in the experiment. Based on TRW's discussion of the effect of changing X_C on laser power, it was inferred that a stable resonator was used. Since BLAZE II uses a Fabry-Perot resonator, which does not include the upstream-downstream coupling present in stable resonators, the BLAZE II model will tend to overpredict the laser performance.

Since a stable resonator was most likely used, and since TRW reported their power spectra at an X_C of 3.5 cm downstream from the nozzle exit plane, some uncertainty exists as to where to stop the lasing calculation. When

BLAZE II was allowed to run the Fabry-Perot calculation to cutoff, the lasing cutoff occurred at 22.6 cm downstream from the nozzle exit plane. Since the mirrors used in the experiment were only 10 cm by 10 cm, it is unlikely that all of the power was measured in the experiment. To better simulate the experiment, the power calculation can be stopped at 2 X_C downstream from the nozzle exit plane, which is 7 cm in this case. The BLAZE II power predictions for lasing to 2 X_C and to cutoff are compared to the RESALE-3 predictions and experimental data in Table 3.

The prediction from BLAZE II is much closer to the experimental results than TRW's original RESALE-3 prediction, but still differs significantly from the experimental results. It is unclear whether the discrepancies are due to errors in the modeling or to errors in the initial conditions assumed for the calculation to fill in gaps in the initial data.

To determine whether or not the inclusion of the collisional decomposition reactions was responsible for the dramatic reduction in predicted power, the BLAZE II calculation was repeated with identical input conditions but with the reaction rates for all of the collisional decomposition reactions zeroed. The resulting total power and vibrational band powers are compared to the experimental results and RESALE-3 calculations in Table 3.

Table 3. Comparison of measured and predicted powers for the TRW baseline chain laser experiment, with and without the collisional decomposition reactions.

Vibrational Band	TRW Experiment[1], Power (W)	RESALE-3, Power[1] (W)	UIUC BLAZE II, to 2X_C (7 cm) Power (W)	UIUC BLAZE II, to cutoff (31.4 cm) Power (W)	UIUC BLAZE II, to 2X_C (7 cm) Power (W) w/ collisional decomposition reactions zeroed	UIUC BLAZE II, to cutoff (39.6 cm) Power (W) w/ collisional decomposition reactions zeroed
P_{10}	12	330	27.1	27.1	27.1	27.1
P_{21}	52.8	960	50.9	50.9	51.8	51.8
P_{32}	42	600	68.0	225	103	807
P_{43}	12	420	6.38	27.2	45.1	558
P_{54}	1.2	360	16.7	181	41.5	682
P_{65}	0	210	15.4	253	26.6	581
P_{76}	0	120	0	0	0	0
P_{total}	120	3000	184	764	295.1	2706.4

The BLAZE II Fabry-Perot calculation did not reach cutoff until 39.6 cm downstream from the nozzle exit plane. Although the predicted power is much greater than that with the collisional decomposition reactions included, it still falls somewhat short of the power predicted by RESALE-3. TRW reported that RESALE-3 predicted 6000 watts of power for a Fabry-Perot calculation that was carried out to 17 cm downstream from the nozzle exit plane. The total power of 3000 watts and respective band powers shown in Table 3 are for a RESALE-3 prediction using the conditions of the experiment, according to TRW. However, since RESALE-3 uses a Fabry-Perot calculation, it is unclear what changes TRW made to the input parameters for their RESALE-3 run to predict 3000 watts. The missing input parameters prevent a resolution between the differences in the predictions by BLAZE II in the present study and the experimental results of TRW. However, the fact that zeroing the collisional decomposition reactions resulted in BLAZE II predicting 2706 watts and their inclusion brought the prediction within a factor of six of the data shows the importance of the collisional decomposition reactions. This result suggests that calculations of chain laser performance that include these reactions may be believable.

Lack of initial data precluded any attempt to accurately model the UARL[3] and Gastaud[4] experiments. Consequently, neither series of experiments was modeled in the present study.

3.4 Investigation of the Possibility of Enhancing CL-XI Performance Via the Hot Reaction

3.4.1 Introduction

The CL-XI combustion-driven HF chemical laser is a kilowatt-class laser operating on the cold HF reaction. It burned C_2D_4 and NF_3 in the combustor, with helium as the diluent. This mixture was injected into the laser cavity through the primary nozzles of the CL-XI 2-D parallel slit supersonic nozzle bank. The secondary nozzles flowed a mixture of H_2 and He diluent. The Bell Aerospace Textron computer code "Combustor Nozzle Cavity Diffuser Ejector" (CNCDE), referred to as "Candy", models the laser from the combustor through the ejector[17]. It then passes the values for the flow conditions at the nozzle exit plane to the BLAZE II code, which computes the details of the lasing flow field within the laser cavity and the power.

3.4.2 Determination of the Effect of Combustor Fuel Reduction on α

The objective was to decrease α in the primary stream. A reduction in the flow rate of the C_2D_4 combustor fuel reduces the stagnation temperature in the combustor, which decreases the fluorine dissociation in the combustor, thus decreasing alpha. To determine the sensitivity of α to C_2D_4 flow rate, the C_2D_4 flow rate was reduced by 10%, 20%, 30%, and 50%. CNCDE assumes that α does not change from the nozzle throat to the nozzle exit plane. The code has three possibilities for the variation of α between the combustor exit and the nozzle throat:

1. α is frozen at the value corresponding to the combustor total temperature (alpha frozen or α_F)
2. α varies from the value corresponding to the combustor total temperature to the value dictated by the F-atom recombination reactions at the static temperature of the throat (alpha kinetic or α_K)
3. α varies from the value corresponding to the combustor total temperature to the value corresponding to equilibrium between the F and F_2 at the static temperature of the throat (alpha equilibrium or α_E)

Surface recombination is not included. Because the entrance section of the primary nozzles is fairly short, the value of α should be between α_F and α_K. Thus, the calculations were performed for these two cases. The values of α at the nozzle exit plane (NEP) corresponding to the 0%, 10%, 20%, 30%, and 50% reduction in C_2D_4 flow rate for α_F are given in Table 4, as well as those corresponding to 0%, 10%, 20%, and 30% reduction in C_2D_4 flow rate for α_K. For α_K, the computation for 50% C_2D_4 reduction was not included because 30% reduction of C_2D_4 was sufficient to obtain $\alpha = 0.05$. From Table 4, it is seen that to reduce α to the 0.03 to 0.05 range of the early experiments, a 30-50% reduction in combustor fuel flow rate is required. Table 4 shows that the power is enhanced for the α_K option, but not for the α_F option when the combustor fuel is decreased.

Table 4. Combustor total temperature, total and static temperatures in the primary stream, α at the NEP, fluorine mass flow rates, and laser performance as a function of combustor fuel reduction, using the frozen alpha and alpha kinetic options. S.L. denotes "still lasing".

C_2D_4 Reduction	Combustor Total T_{tPRI} (K)	Primary Total T_{tPRI} (K)	Primary Static T_{static} (K)	α at nozzle exit	$\dot{m}_F$ at nozzle exit (g/s)	$\dot{m}_{F_2}$ at nozzle exit (g/s)	P_{total} (kw)	Lasing Cutoff (cm)	Choking Distance (cm)
α_F Option, Original CL-XI flow channel, 99% reflective mirrors									
0%	1949	1501	160.4	0.988	6.311	0.0736	5.65	3.83	none
10%	1636	1183	114.3	0.909	7.622	0.7590	4.62	2.38	none
20%	1418	967	86.28	0.639	6.634	3.740	3.51	S.L	1.21
30%	1263	816	68.31	0.334	4.137	8.233	2.86	S.L.	1.26
50%	899	461	30.49	0.015	0.2364	16.06	0.68	28.93	none
α_K Option, Original CL-XI flow channel, 99% reflective mirrors									
0%	1949	1599	178.5	0.638	4.076	2.314	5.91	4.11	none
10%	1636	1402	150.0	0.313	2.624	5.761	6.44	4.26	none
20%	1418	1193	121.2	0.125	1.295	9.079	7.84	7.26	none
30%	1263	959	89.14	0.045	0.5555	11.81	7.25	33.48	none

3.4.3 Thermal Choking

When the Mach number of the flow is predicted to approach unity, the BLAZE II code stops the calculation and provides a warning message about thermal choking. The high heat release of the chain reaction induced thermal choking in two of the runs using the original CL-XI flow channel and the α_F option. This is a phenomenon noted earlier by TRW[1], which TRW called "thermal runaway". The flow channel geometry was modified, Fig. 1, to prevent thermal choking. Although the increase in total power due to C_2D_4 flow rate reduction was significant, a larger increase in total power was obtained by changing the flow channel geometry. From Table 5 it is seen that the cases with no reduction in C_2D_4 flow rate were predicted to nearly double in power when the flow channel geometry was changed. This indicates that laser performance may be optimized by proper choice of the flow channel geometry.

3.4.4 Effect of the Hot Reaction

If the HF chain reaction is occurring, the higher vibrational levels of HF populated by the hot reaction, namely HF(v = 3, 4, 5, 6), should be present in some concentration. HF(v) populations are plotted in Figs. 2-4 for 90% mirror reflectivities and the original CL-XI flow channel geometry. The α_F option is used in Fig. 2, while α_K is used in Figs. 3 and 4. No C_2D_4 reduction is used in Figs. 2–3, and a 30% reduction is used in Fig. 4 (see Ref. 16 for details with 10% and 20% reductions).

Table 5. Predicted laser performance using the frozen alpha and alpha kinetic options as a function of flow channel geometry. Conditions for all cases: C_2D_4 Reduction=0%, $T_{t,comb}$ = 1949 K, α at combustor exit = 0.988. Results from Channels 1 and 2 are not listed as they resulted in choked flow, whereas Channels 3 and 4 did not choke.

Channel	P_{total} (kW)	P_{10} (kW)	P_{21} (kW)	P_{32} (kW)	P_{43} (kW)	P_{54} (kW)	P_{65} (kW)	Cutoff (cm)
α_F Option, α at nozzle exit = 0.988, $\dot{m}_F$ at nozzle exit = 6.31 g/s, $\dot{m}_{F_2}$ at nozzle exit = 0.074 g/s								
Original	5.65	2.82	2.69	0.14	0	0	0	3.8
3	10.2	4.91	5.09	0.18	0	0	0	8.8
4	10.7	4.93	5.57	0.17	0	0	0	14.2
α_K Option, α at nozzle exit = 0.638, $\dot{m}_F$ at nozzle exit = 4.08 g/s, $\dot{m}_{F_2}$ at nozzle exit = 2.31 g/s								
Original	5.91	2.90	2.86	0.13	0	0.013	0	4.1
3	10.8	5.20	5.42	0.19	0	0	0	8.6
4	10.7	4.93	5.57	0.17	0	0	0	14.2

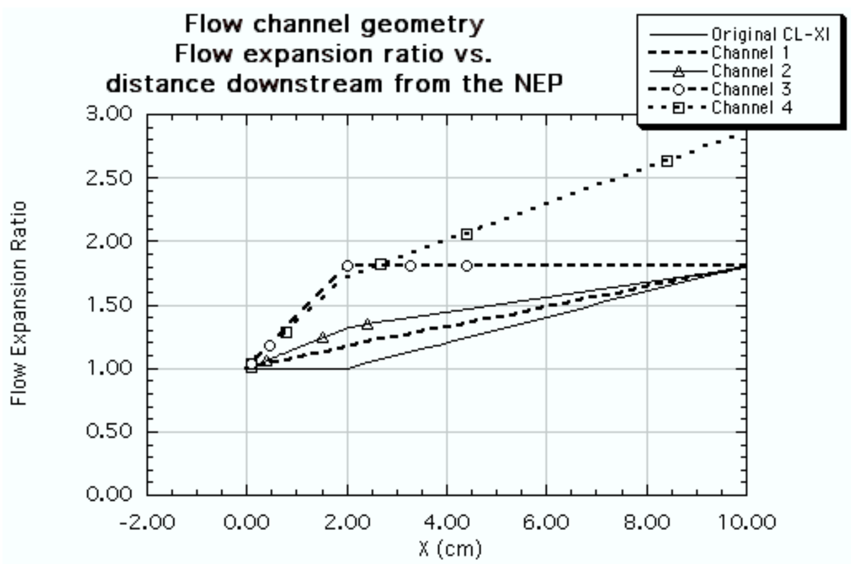

Figure 1. Flow channel geometry as a function of downstream distance for five flow channel geometries $\left(\text{flow expansion ratio} = \dfrac{\text{channel height}}{\text{nozzle bank height}}\right)$.

Comparison of the run with reduced C_2D_4 flow rate (Fig. 4) to the run with no C_2D_4 reduction (Fig. 3) shows that reduced C_2D_4 flow rates increased the initial concentration of excited HF(v ≥ 3) and reduced the concentration of HF in lower vibrational states downstream from the NEP. Near the NEP, the mole mass ratios of HF(v) do not change significantly between runs. This established that the chain reaction was occurring.

To determine the influence of the hot reaction, the calculations were repeated with the hot pumping reactions removed, Eq. (2). By setting the rate coefficients for each v in Eq. (2) equal to zero in BLAZE II, the effects of the hot reaction are removed from the calculations. The resulting mole/mass ratios of HF(v) are plotted in Figs. 5-7. These figures demonstrate that the hot reaction is no longer populating the upper vibrational levels.

HF(4) is produced in small amounts by reactions (8)-(13). This is probably due to the fact that the mole mass ratios of the lower vibrational levels of HF are several orders of magnitude larger than mole mass ratio of HF(4), which shifts the reaction equilibrium toward the reverse direction.

$$HF(4) + M \Leftrightarrow HF(3) + M \quad (8)$$

$$HF(4) + M \Leftrightarrow HF(2) + M \quad (9)$$

$$HF(4) + M \Leftrightarrow HF(1) + M \quad (10)$$

$$HF(2) + HF(4) \Leftrightarrow HF(3) + HF(3) \quad (11)$$

$$HF(0) + HF(4) \Leftrightarrow HF(1) + HF(3) \quad (12)$$

$$HF(1) + HF(4) \Leftrightarrow HF(2) + HF(3) \quad (13)$$

Although mole/mass ratios of HF(v = 0, 1, 2, 3) in the runs with the hot reaction zeroed are nearly identical to their counterpart in runs with the hot reaction included, these mole mass ratios are noticeably smaller as one moves downstream in the case with the hot reaction zeroed. This is true even in the case when there was no reduction of the combustor fuel. This is probably because the excited HF generated by the hot reaction, after being collisionally decomposed by H, would produce H_2 and F, which react to populate the vibrational levels pumped by the cold reaction.

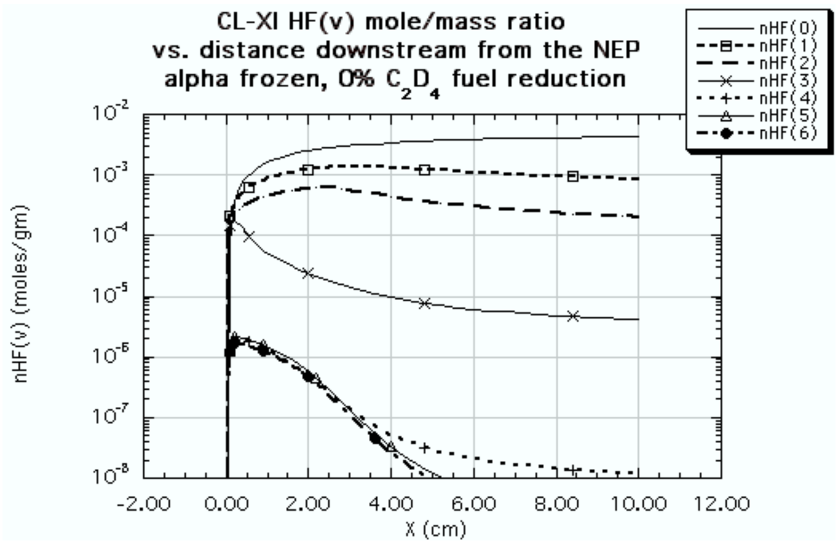

Figure 2. Mole/mass ratio of excited HF(v) vs. distance downstream from the NEP, 0% combustor fuel reduction. Associated conditions: alpha frozen, 90% mirror reflectivities, original CL-XI flow channel geometry.

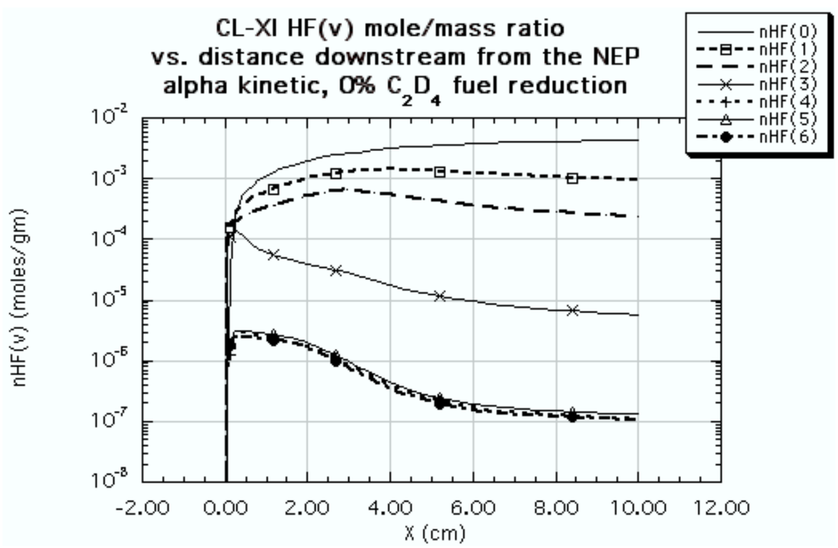

Figure 3. Mole/mass ratio of excited HF(v) vs. distance downstream from the NEP, 0% combustor fuel reduction. Associated conditions: alpha kinetic, 90% mirror reflectivities, original CL-XI flow channel geometry.

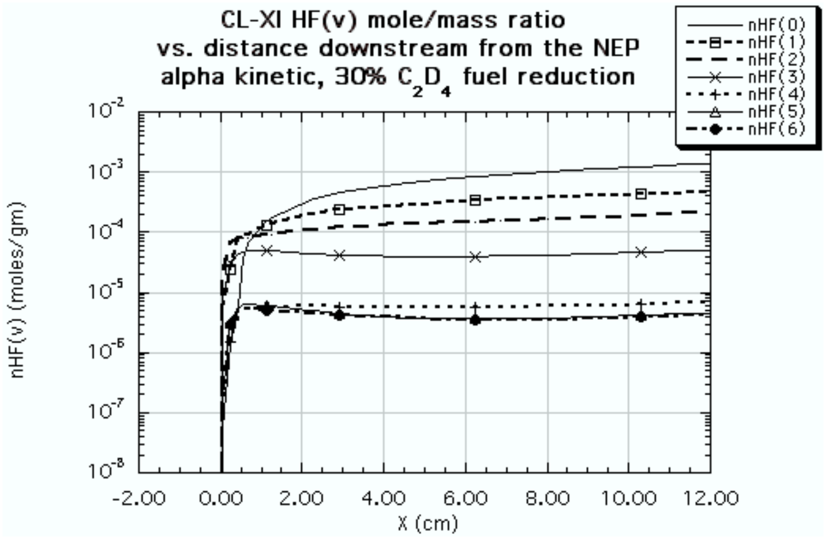

Figure 4. Mole/mass ratio of excited HF(v) vs. distance downstream from the NEP, 30% combustor fuel reduction. Associated conditions: alpha kinetic, 90% mirror reflectivities, original CL-XI flow channel geometry.

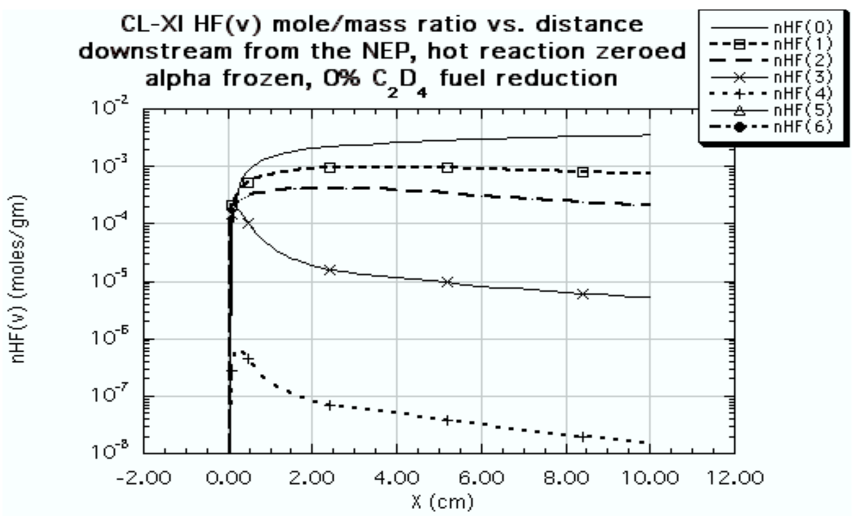

Figure 5. Mole/mass ratio of excited HF(v) vs distance downstream from the NEP, hot pumping reactions zeroed, 0% combustor fuel reduction. Associated conditions: alpha frozen, 90% mirror reflectivities, original CL-XI flow channel geometry.

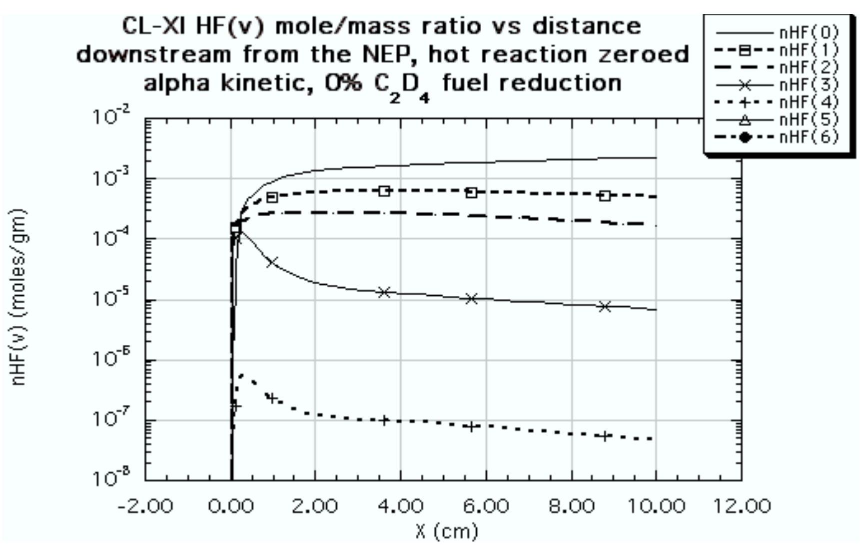

Figure 6. Mole/mass ratio of excited HF(v) vs distance downstream from the NEP, hot pumping reactions zeroed, 0% combustor fuel reduction. Associated conditions: alpha kinetic, 90% mirror reflectivities, original CL-XI flow channel geometry.

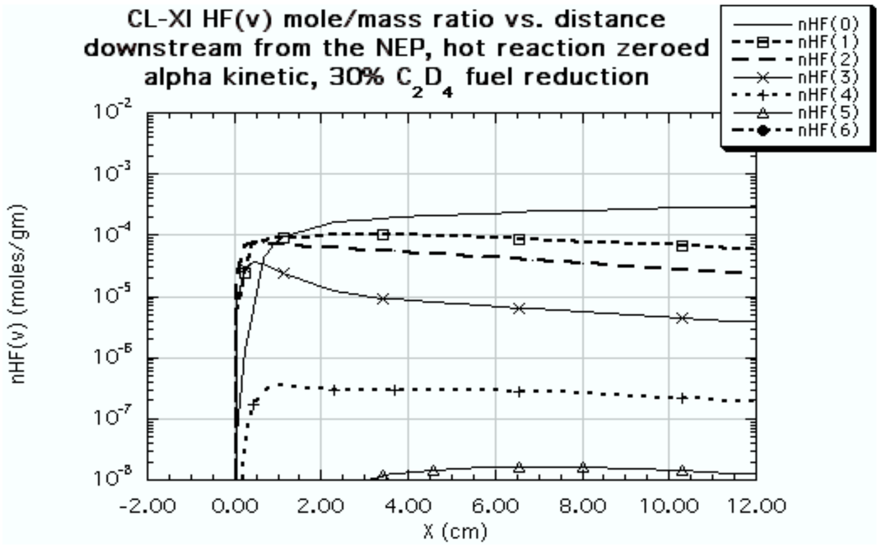

Figure 7. Mole/mass ratio of excited HF(v) vs distance downstream from the NEP, hot pumping reactions zeroed, 30% combustor fuel reduction. Associated conditions: alpha kinetic, 90% mirror reflectivities, original CL-XI flow channel geometry.

3.4.5 Additional Power Generation by the Chain Reaction

The most important question to be answered by this study is whether or not additional power can be obtained from a cw HF laser by running on the hot reaction. To answer this question, power calculations were performed for the chain-reaction CL-XI laser. The results using the α_F option did not appear promising, Table 4 (see Ref. 16 for details). In each case, reducing the level of C_2D_4 flow rate below the original flow rate produced a total power drop.

The results using the α_K option are in sharp contrast to those using α_F, Table 4. Increases in total power between 9% and 33% are predicted for some level of C_2D_4 reduction with 99% mirror reflectivities. The hot reaction provided the greatest performance increase when the media was highly saturated.[16] The total power levels for runs using the α_K option suggest that reduction of alpha in HF lasers may result in 10% to 30% additional power.

The question of how much of the power was generated by the hot reaction can be answered by examining the calculations conducted with the hot pumping reaction zeroed. The "change in total power" is obtained by comparing power calculations with and without the hot pumping reactions. The change in total power, which is calculated as,

$$(\text{change in total power}) = \frac{\begin{pmatrix}\text{total power with}\\ \text{hot reaction zeroed}\end{pmatrix} - \begin{pmatrix}\text{total power including}\\ \text{hot reaction}\end{pmatrix}}{(\text{total power including hot reaction})} \qquad (14)$$

is summarized in Table 5. Zeroing the hot reaction produced a loss of power for two cases using α_F, and substantial losses of power for every case using α_K. In only one case did zeroing the hot reaction cause an increase in power, albeit a small increase. For both α_F and α_K, the magnitude of the loss of power with the hot reaction zeroed increases with increasing C_2D_4 flow rate reduction. Since the cases with no reduction in C_2D_4 flow rate lost power when the hot reaction was zeroed, the chain reaction is actually responsible for a portion of the power generated by lasers which are designed to run on the cold reaction.

Table 5. Effect of hot pumping reaction on CL-XI performance as a function of C_2D_4 flow rate reduction for 90% mirror reflectivities, for α_F and for α_K option.

C_2D_4 reduction	Change in total power when hot reaction is zeroed (%) for α_F option	Change in total power when hot reaction is zeroed (%) for α_K option
0%	-1.78%	-17.20%
10%	2.38%	-42.7%
20%	0%	-72.79%
30%	-16.88%	-85.03%

3.4.6 F_2 Injection

The preceding calculations showed that reduction of the C_2D_4 flow rate reduced α and, under certain conditions, resulted in an increase in HF laser power. Since injection of F_2 at the exit of the primary nozzle will also reduce α, calculations were performed to determine if such injection results in an increase in CL-XI power. The injection of F_2 was tried for both the α_F and α_K cases with 0% C_2D_4 reduction. The results are given in Table 6 for α_F and α_K.

In the α_F case, injection of F_2 reduces the total power of the laser, but not as much as when the C_2D_4 flow rate is reduced to achieve an equivalent α. In the α_K case, injection of F_2 increases the total power, but not as much as when the C_2D_4 flow rate is reduced to obtain the same α.

For the α_F case, 3.7 g/s of F_2 injection brought the F and F_2 flow rates of the laser to approximately the F and F_2 flow rates for the α_F case with 20% C_2D_4 reduction. However, the case with 20% C_2D_4 reduction choked, whereas the case with 3.7 g/s F_2 injection did not. Injection of 0.323 g/s of F to obtain an exact match between the F and F_2 flow rates of the two cases had little effect on the performance, as it only reduced the total power by 1.5% and did not cause the flow to choke. It was noticed that the static and total temperatures of the primary stream were greater in the case with F_2 injection. When the static temperature of the primary stream was reduced to 86.3 K to match the static temperature in the 20% C_2D_4 reduction case, the flow choked and the total power of the laser was within 4% the 20% C_2D_4 reduction case. Reduction of the static temperature in the primary stream brought the total temperature in the primary stream down to 847 K, within 12% of the 20% C_2D_4 reduction case's value of 967 K. Reduction of the static and total temperature of the primary stream promoted thermal choking and reduced the total power output of the laser.

For the case with α_K, 3.45 g/s of F_2 injection brought the F_2 flow rate into agreement with the α_K 10% C_2D_4 reduction case. However, the flow choked and produced less power than the case with no F_2 injection. The flow rate of F in the case with F_2 injection was much higher than in the case with 10% C_2D_4 reduction. When the F flow rate was reduced to the level of the 10% C_2D_4 reduction case, choking did not occur. The laser performance is sensitive not only to the F_2 flow rate in the primary stream, but also to the F flow rate. The power in the case with the F and F_2 flow rates matched to those of the 10% C_2D_4 reduction case is greater than the power in the case with 10% C_2D_4 reduction, Table 6. Reduction of the static temperature in the primary stream to 150 K to match that of the 10% C_2D_4 reduction case resulted in a predicted total power that is too low. Although the static temperature of the primary streams at the NEP in the two cases were matched, the total temperature of the primary stream in the F_2 injection case was 1343 K, which is 59 K lower than the 1402 K total temperature in the primary stream of the 10% C_2D_4 reduction case. Increasing the static temperature of the primary stream by 10% in the F_2 injection case resulted in a close match in total power between the two cases.

Since the performance of F_2 injection runs matched the performance of C_2D_4 reduction runs with similar α only when the total temperature in the primary stream of the two runs matched, the difference in performance between α_F runs and α_K runs with similar α may be explained by differences in total temperature in the primary streams. For the α_F case, it was necessary to reduce the C_2D_4 flow rate, and thus the total temperature of the flow in the primary stream, to a larger extent than for the α_K case to achieve the same value of α in the flow. Therefore, in cases with similar α, an α_F case had a lower total temperature in the primary stream than an α_K case. In the F_2 injection cases above, lower total temperatures in the primary stream resulted in thermal choking and less total power. In α_F C_2D_4 reduction cases, power was lower than in the α_K cases and thermal choking occurred. The dependence of total power and thermal choking in F_2 injection cases on the primary stream total temperature explains the differences in total power and thermal choking between the α_F and α_K C_2D_4 reduction cases.

Table 6. Combustor total temperature, α, fluorine mass flow rates in the primary nozzle, and laser performance as a function of combustor fuel reduction for α_F and for α_K options. S.L. denotes "still lasing".

F_2 inj. (g / sec)	F inj. (g / sec)	Primary Total T_{tPRI} (K)	Primary Static T_{static} (K)	α at nozzle exit	$\dot{m}_F$ at nozzle exit (g/s)	$\dot{m}_{F_2}$ at nozzle exit (g/s)	P_{total} (kw)	Lasing Cutoff (cm)	Choking Distance (cm)
α_F Option, Original CL-XI flow channel, 99% reflective mirrors									
0	0	1501	160.4	0.988	6.311	0.0736	5.65	3.83	none
2	0	1492	160.4	0.753	6.311	2.0736	5.44	2.64	none
3.7	0	1484	160.4	0.626	6.311	3.7736	5.32	2.03	none
3.7	0.323	1485	160.4	0.639	6.634	3.740	5.24	1.88	none
3.7	0.323	847	86.3	0.639	6.634	3.740	3.37	S.L.	1.057
5	0	1478	160.4	0.554	6.311	5.0736	5.23	1.638	1.639
α_K Option, Original CL-XI flow channel, 99% reflective mirrors									
0	0	1599	178.5	0.638	4.076	2.314	5.91	4.11	none
2	0	1589	178.5	0.486	4.076	4.314	6.00	3.045	none
3.45	0	1582	178.5	0.414	4.076	5.761	6.03	2.510	none
3.45	0	1348	150.0	0.414	4.076	5.761	5.51	S.L.	2.209
3.45	-1.46	1576	178.5	0.313	2.62	5.761	6.68	4.086	none

3.45	-1.46	1466	165.0	0.313	2.62	5.761	6.40	3.958	none
3.45	-1.46	1343	150.0	0.313	2.62	5.761	6.09	3.787	none
5	0	1575	178.5	0.358	4.076	7.314	5.99	S.L.	2.03

IV. CONCLUDING REMARKS

The goals of this study were to determine if it is possible to obtain additional power from cw HF lasers by utilizing the HF hot reaction and, if so, under what conditions this additional power may be obtained.

Computational models were employed by TRW[1], UARL[3], and Bell Aerospace Textron[5] to predict performance of lasers that employ the HF hot reaction. Because these models did not include the collisional decomposition of HF($v \geq 3$) by H atoms, these models overpredicted performance by a factor of 15 to 30. To determine if the inclusion of the collisional decomposition reactions would improve the agreement of the models with experiment, the chain reaction laser experiment of TRW was modeled using the BLAZE II rotational equilibrium code[6] with the collisional decomposition of HF($v \geq 3$) by H atoms included. Inclusion of these reactions resulted in a power prediction that is within a factor of six of TRW's experimental results. Better agreement could not be obtained because too few details about the conditions of TRW's experiment were given in the references.

The CL-XI combustion-driven laser[7] was modeled using BLAZE II with the collisional decomposition reactions included. Reduction of the C_2D_4 combustor fuel flow rate reduced the combustor total temperature and reduced α of the primary flow. Reduction of the C_2D_4 flow rate resulted in a performance increase of 10 to 30% provided that the F atom recombination kinetics form F_2 between the combustor and the NEP. If α in the primary stream is frozen from the combustor exit to the NEP, reducing the C_2D_4 flow rate did not result in an increase in power—in fact, it resulted in a decrease.

To determine how much of the predicted CL-XI power was generated by the HF hot reaction, the hot reactions were zeroed in the BLAZE II model. Several of the CL-XI runs with and without C_2D_4 reduction were repeated with the hot reactions zeroed. In the cases with no C_2D_4 reduction, the hot reactions were responsible for 2% of the power for α_F cases and for 17% of the power for α_K cases. This suggests that the hot reactions contribute to combustion driven laser performance in lasers designed to operate on the HF cold reaction by 2 - 17%. For the cases with C_2D_4 reduction, the hot reactions were responsible for increasing percentages of the power with increasing C_2D_4 reduction. The hot reactions were responsible for less than 17% of the power in α_F runs, and for 20% to 85% of the power in α_K runs.

For both the arc and combustion driven lasers, the higher the medium saturation, the larger the percent increase in power due to the hot reaction. This is likely a result of lower gains on the higher vibrational bands.

These results show that four conditions are necessary to obtain increased laser performance from the HF hot reaction:

1. reduced fluorine dissociation at the primary nozzle exit plane;
2. the correct total temperature of the primary flow;
3. proper design of the laser cavity flow channel geometry;
4. the medium must be well saturated.

All four of these conditions must be optimized together to obtain increased laser performance from the hot reaction. Satisfying one or two of these by themselves is not sufficient.

Since the computational results of this study suggest that significant increases in laser performance may be obtained from the HF hot reaction, and from optimization of the laser cavity flow channel geometry, appropriate experiments should be performed to verify these results.

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