



AIAA 2002-2277

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33rd Plasmadynamics and Lasers Conference

20-23 May 2002

Maui, Hawaii

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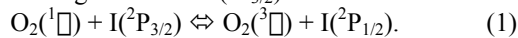
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Abstract

Theoretical studies have indicated that fractions of $O_2(^1\Sigma)$ may be produced in an electrical discharge that will permit lasing of an ElectriCOIL system in conjunction with injection of pre-dissociated iodine. Results of those studies along with more recent experimental results show that electric excitation is a very complicated process that must be investigated with advanced diagnostics along with modeling to better understand this highly complex system. In this paper, experimental data and output from the detailed electrodynamic GlobalKin model are used as input for the Blaze II laser modeling code to better understand how to guide future experiments towards a laser demonstration. A kinetic package appropriate for the ElectriCOIL system is presented. Gain, specie, and temperature plots are provided for a preliminary parametric study.

1.0 Introduction

The classic chemical oxygen-iodine laser (COIL) [McDermott, 1978] operates on the electronic transition of the iodine atom at 1315 nm, $I(^2P_{1/2}) \rightarrow I(^2P_{3/2}) + h\nu$. The population inversion is obtained by a near resonant energy transfer between the excited $O_2(^1\Sigma)$ molecule and the I atom ground state $I(^2P_{3/2})$ via



Traditionally, this pumping reaction is fed by a liquid chemistry singlet oxygen generator (SOG). However, the logistic issues of dealing with the liquid SOG

systems motivated the investigation of excitation of iodine via all gas phase means by various research groups. AFRL recently demonstrated a new all gas phase iodine laser fed by the $NCI(^1\Sigma)$ molecule [Henshaw, 2000]. We believe that it is possible to construct a highly efficient electric generation scheme to provide the precursor energy donor species $O_2(^1\Sigma)$ and that an electrically assisted COIL system (ElectriCOIL) [Carroll, 2001; King, 2001; Verdeyen, 2002] can be realized. Researchers at CU Aerospace (CUA) and the University of Illinois at Urbana-Champaign (UIUC) are now addressing the scientific and engineering issues associated with this concept.

Researchers around the world have previously shown that flowing discharge tubes containing ground state oxygen can produce significant quantities of the desired $O_2(^1\Sigma)$ precursor molecules. Benard and Pchelkin [Benard, 1978] reported 11% yield using a microwave discharge. Fujii [Fujii, 1994] reported good success, 17% yield of $O_2(^1\Sigma)$, with a small RF generator. More recently, workers in Japan [Itami, 1999] from Fujisaki Electric provided some evidence that they could produce 21% $O_2(^1\Sigma)$ in a microwave discharge. Hill [Hill, 2001] reported a value of 16% with a controlled-avalanche discharge scheme. Schmiedberger [Schmiedberger, 2001] reported a 32% yield under low-pressure conditions (0.43 Torr) with an RF discharge. We have recently obtained an $O_2(^1\Sigma)$ yield of $\approx 16\%$ in our flowing RF discharge experiments at a pressure of 2 Torr [Verdeyen, 2002].

Since the yields of $O_2(^1\Sigma)$ using electrical excitation appears to be lower than those with the classic liquid SOG method, it was determined in the original ElectriCOIL concept [Carroll, 2001] that atomic iodine injection, rather than molecular iodine injection, will be an important, if not essential, addition to boosting performance of the ElectriCOIL laser. Experimental work in the area of iodine pre-dissociation has been conducted by Endo and Fujioka's group in Japan [Endo, 1999]. They reported nearly total dissociation from interaction of an Iodine/ N_2 stream

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within the microwave cavity. Iodine pre-dissociation has also been investigated using 3-dimensional CFD computations by Madden *et al.* [Madden, 1998]; Madden's results indicated that the injection of atomic iodine slightly downstream of the throat would enhance the power output of a classic COIL device. Recently, CUA and UIUC implemented an LIF experiment that showed 50% dissociation downstream from a DC electric discharge and about 95% in an RF discharge [Verdeyen, 2002].

2.0 Preliminary System Studies

The limitations of existing COIL technology as well as the possible improvement from the implementation of ElectriCOIL technology are illustrated in Figure 1.

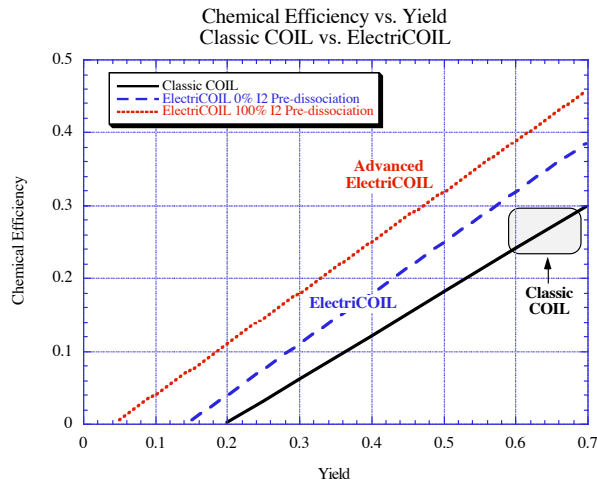


Figure 1. A comparison between classic COIL technology and the performance possibilities for an ElectriCOIL device. Results based upon a heuristic equation [Hon, 1996] at a laser cavity temperature of 150 K.

We choose chemical efficiency as a way of relating classic COIL performance to the ElectriCOIL concept. In a classic COIL system, the chemical efficiency is defined by

$$\eta_{chem, classic} = \frac{P_{out}}{91 \dot{n}_{Cl_2}}, \quad (2)$$

where P_{out} is the outcoupled laser power in kW, \dot{n}_{Cl_2} is the chlorine flow rate in moles/s, and the factor 91 is the amount of energy contained by 1 mole of the lasing transition of iodine atoms in kJ. In classic COIL, the chlorine is mostly converted to oxygen in the SOG. For an ElectriCOIL device there is no chlorine, therefore, for comparison purposes we define the ElectriCOIL chemical efficiency to be

$$\eta_{chem, ElectriCOIL} = \frac{P_{out}}{91 \dot{n}_{O_2}}, \quad (3)$$

where \dot{n}_{O_2} is the oxygen flow rate in moles/s (note that this is equivalent to the classic COIL definition with 100% utilization of the chlorine).

Elimination of the aqueous SOG in a classic COIL system represents a significant reduction in system weight, along with simpler operation procedures; Figure 1 indicates that even an ElectriCOIL that provides 20% chemical efficiency is an enormous improvement to the classic COIL design.

3.0 Kinetic Mechanism

Ongoing ElectriCOIL experiments along with recent GlobalKin [Dorai, 2001] simulations have indicated that the kinetic processes taking place in the ElectriCOIL flow system are extremely complex, especially in the discharge region. GlobalKin results indicate the production of atomic oxygen in the discharge region with exit concentrations on the order of those of the $O_2(^1\Sigma)$; this result is consistent with the experimental measurements by Ivanov *et al.* [Ivanov, 1999]. Other GlobalKin results show that significant quantities of $O_2(^1\Sigma)$ are produced in the discharge along with small, but possibly important, levels of O_3 . Discussions with Heaven [Heaven, 2001] suggested the need to incorporate reactions between molecular iodine and atomic oxygen as being an important process. Research by Schmiedberger [Schmiedberger, 2001] indicates the use of NO and/or NO_2 as being potentially important for enhancing the production of $O_2(^1\Sigma)$. Lastly, there is the desire to perform and model titrations with gases such as NO_2 for O atoms and CO_2 for $O_2(^1\Sigma)$. As such, it is necessary to expand the classic COIL reaction set that is included in the Blaze II model. Table 1 presents the classic COIL reaction set used in Blaze II, and Table 2 presents the expanded mechanism used for the Blaze II modeling of the ElectriCOIL system. Note that the rate for reaction 57 is unknown (zero is presently used as the rate), but the reaction could potentially be important and so is noted in the mechanism.

Table 1. Classic COIL reaction set. Note: I represents the $I(^2P_{3/2})$ state, I^* the $I(^2P_{1/2})$ state, and I_2^* is $I_2(v>40)$.
 Reactions 16-20 were taken from discussions with Heaven, 1996, based upon data from Lawrence, 1997.

k							Rates, $\text{cm}^3/\text{molecule-s}$	Ref.	
1	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^1\Pi)$	\rightarrow	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^3\Pi)$	2.7e-17	Perram, 1988
2	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^1\Pi)$	\rightarrow	$\text{O}_2(^3\Pi)$	+	$\text{O}_2(^3\Pi)$	1.7e-17	Perram, 1988
3	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^3\Pi)$	\rightarrow	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^3\Pi)$	3.9e-17	Perram, 1988
4	$\text{O}_2(^1\Pi)$	+	H_2O	\rightarrow	$\text{O}_2(^1\Pi)$	+	H_2O	6.7e-12	Perram, 1988
5	$\text{O}_2(^1\Pi)$	+	Cl_2	\rightarrow	$\text{O}_2(^1\Pi)$	+	Cl_2	2.0e-15	Perram, 1988
6	$\text{O}_2(^1\Pi)$	+	He	\rightarrow	$\text{O}_2(^1\Pi)$	+	He	1.0e-17	Perram, 1988
7	$\text{O}_2(^1\Pi)$	+	$\text{O}_2(^3\Pi)$	\rightarrow	$\text{O}_2(^3\Pi)$	+	$\text{O}_2(^3\Pi)$	1.6e-18	Perram, 1988
8	$\text{O}_2(^1\Pi)$	+	H_2O	\rightarrow	$\text{O}_2(^3\Pi)$	+	H_2O	4.0e-18	Perram, 1988
9	$\text{O}_2(^1\Pi)$	+	Cl_2	\rightarrow	$\text{O}_2(^3\Pi)$	+	Cl_2	6.0e-18	Perram, 1988
10	$\text{O}_2(^1\Pi)$	+	He	\rightarrow	$\text{O}_2(^3\Pi)$	+	He	8.0e-21	Perram, 1988
11	I_2	+	$\text{O}_2(^1\Pi)$	\rightarrow	2I	+	$\text{O}_2(^3\Pi)$	4.0e-12	Perram, 1988
12	I_2	+	$\text{O}_2(^1\Pi)$	\rightarrow	I_2	+	$\text{O}_2(^3\Pi)$	1.6e-11	Perram, 1988
13	I_2	+	$\text{O}_2(^1\Pi)$	\rightarrow	I_2^*	+	$\text{O}_2(^3\Pi)$	7.0e-15	Perram, 1988
14	I_2	+	I^*	\rightarrow	I	+	I_2^*	3.5e-11	Perram, 1988
15	I_2^*	+	$\text{O}_2(^1\Pi)$	\rightarrow	2I	+	$\text{O}_2(^3\Pi)$	3.0e-10	Perram, 1988
16	I_2^*	+	$\text{O}_2(^3\Pi)$	\rightarrow	I_2	+	$\text{O}_2(^3\Pi)$	4.9e-12	Lawrence, 1997
17	I_2^*	+	H_2O	\rightarrow	I_2	+	H_2O	1.7e-11	Lawrence, 1997
18	I_2^*	+	He	\rightarrow	I_2	+	He	9.8e-12	Lawrence, 1997
19	I_2^*	+	Cl_2	\rightarrow	I_2	+	Cl_2	6.3e-12	Lawrence, 1997
20	I_2^*	+	N_2	\rightarrow	I_2	+	N_2	8.2e-12	Lawrence, 1997
21	I	+	$\text{O}_2(^1\Pi)$	\rightarrow	I^*	+	$\text{O}_2(^3\Pi)$	7.8e-11	Perram, 1988
22	I^*	+	$\text{O}_2(^3\Pi)$	\rightarrow	I	+	$\text{O}_2(^1\Pi)$	1.04e-10*exp(-401.4/T)	Perram, 1988
23	I	+	$\text{O}_2(^1\Pi)$	\rightarrow	I	+	$\text{O}_2(^3\Pi)$	1.0e-15	Perram, 1988
24	I^*	+	$\text{O}_2(^3\Pi)$	\rightarrow	I	+	$\text{O}_2(^3\Pi)$	3.5e-16	Perram, 1988
25	I^*	+	$\text{O}_2(^1\Pi)$	\rightarrow	I	+	$\text{O}_2(^1\Pi)$	1.0e-13	Perram, 1988
26	I^*	+	$\text{O}_2(^1\Pi)$	\rightarrow	I	+	$\text{O}_2(^1\Pi)$	1.1e-13	Perram, 1988
27	I^*	+	I	\rightarrow	I	+	I	1.7e-13	Perram, 1988
28	I^*	+	H_2O	\rightarrow	I	+	H_2O	2.1e-12	Perram, 1988
29	I^*	+	He	\rightarrow	I	+	He	5.0e-18	Perram, 1988
30	I^*	+	N_2	\rightarrow	I	+	N_2	5.0e-18	Estimated
31	I^*	+	Cl_2	\rightarrow	Cl	+	ICl	5.5e-15	Perram, 1988
32	I^*	+	Cl_2	\rightarrow	I	+	Cl_2	8.0e-15	Perram, 1988
33	I^*	+	ICl	\rightarrow	I_2	+	Cl	1.5e-11	Perram, 1988
34	I_2	+	Cl	\rightarrow	I	+	ICl	2.0e-10	Perram, 1988
35	Cl	+	ICl	\rightarrow	I	+	Cl_2	8.0e-12	Perram, 1988
36	2I	+	I_2	\rightarrow	I_2	+	I_2	3.6e-30	Perram, 1988
37	2I	+	He	\rightarrow	I_2	+	He	3.8e-33	Busch, 1981
38	2I	+	N_2	\rightarrow	I_2	+	N_2	4.2e-32	Busch, 1981
39	$\text{I}^* + \text{I}$	+	I_2	\rightarrow	$\text{I}_2(\text{B})$	+	I_2	3.6e-30	Perram, 1988
40	$\text{I}_2(\text{B})$			\rightarrow	2I			1.0e+6	Perram, 1988

Table 2. Additional ElectriCOIL related reactions.

k							Rates, cm ³ /molecule-s	Ref.	
41	2O	+	He	→	O ₂ (³ □)	+	He	5.2e-35	Kushner, 2001
42	2O	+	O ₂ (³ □)	→	O ₂ (³ □)	+	O ₂ (³ □)	5.2e-35	Kushner, 2001
43	2O	+	O ₂ (¹ □)	→	O ₂ (³ □)	+	O ₂ (¹ □)	5.2e-35	Kushner, 2001
44	2O	+	O	→	O ₂ (³ □)	+	O	5.2e-35	Kushner, 2001
45	O + O ₂ (³ □)	+	He	→	O ₃	+	He	6.0e-34*(T/300) ^{-2.8}	Atkinson, 1997
46	O + O ₂ (³ □)	+	O ₂ (³ □)	→	O ₃	+	O ₂ (³ □)	6.0e-34*(T/300) ^{-2.8}	Atkinson, 1997
47	O + O ₂ (³ □)	+	O ₂ (¹ □)	→	O ₃	+	O ₂ (¹ □)	6.0e-34*(T/300) ^{-2.8}	Atkinson, 1997
48	O + O ₂ (³ □)	+	O	→	O ₃	+	O	6.0e-34*(T/300) ^{-2.8}	Atkinson, 1997
49	O ₂ (¹ □)	+	O	→	O ₂ (¹ □)	+	O	7.2e-14	Atkinson, 1997
50	O ₂ (¹ □)	+	O	→	O ₂ (³ □)	+	O	0.8e-14	Atkinson, 1997
51	O ₂ (v)	+	O ₂ (³ □)	→	O ₂ (³ □)	+	O ₂ (³ □)	1.0e-14*sqrt(T/300)	Kushner, 2001
52	O ₂ (v)	+	He	→	O ₂ (³ □)	+	He	1.0e-14*sqrt(T/300)	Kushner, 2001
53	O	+	O ₃	→	O ₂ (³ □)	+	O ₂ (³ □)	8.0e-12*exp(-2060/T)	Atkinson, 1997
54	O ₂ (¹ □)	+	O ₃	→	2O ₂ (³ □)	+	O	5.2e-11*exp(-2840/T)	Atkinson, 1997
55	I ₂	+	O	→	IO	+	I	1.4e-10	Atkinson, 1997
56	IO	+	O	→	I	+	O ₂ (³ □)	3.0e-11	Atkinson, 1997
57	I*	+	O	→	I	+	O	unknown	
58	O	+	NO ₂	→	NO	+	O ₂ (³ □)	6.5e-12*exp(120/T)	Atkinson, 1997
59	O	+	NO	→	NO ₂			2.5e-17	Kaufman, 1958
60	O + NO	+	O ₂ (³ □)	→	NO ₂	+	O ₂ (³ □)	1.0e-31*(T/300) ^{-1.5}	Atkinson, 1997
61	O*	+	O ₂ (³ □)	→	O	+	O ₂ (¹ □)	2.56e-11*exp(67/T)	Atkinson, 1997
62	O*	+	O ₂ (³ □)	→	O	+	O ₂ (¹ □)	0.16e-11*exp(67/T)	Atkinson, 1997
63	O*	+	O ₂ (³ □)	→	O	+	O ₂ (³ □)	0.48e-11*exp(67/T)	Atkinson, 1997
64	O*	+	O ₃	→	2O	+	O ₂ (³ □)	1.2e-10	Atkinson, 1997
65	O*	+	O ₃	→	O ₂ (³ □)	+	O ₂ (³ □)	1.2e-10	Atkinson, 1997
66	O ₂ (¹ □)	+	CO ₂	→	O ₂ (¹ □)	+	CO ₂	4.1e-13	Atkinson, 1997

4.0 Subsonic Studies

The Blaze II laser simulation code [Sentman, 1977] contains one-dimensional fluid dynamic equations whose mixing terms were derived from the two-dimensional equations that describe the mixing flowfield in a chemical laser cavity. The model can be used for premixed, axisymmetric and two-dimensional flows and has proven to be a robust and useful modeling tool for 25 years for several different types of chemical lasers. The use of this model for COIL simulations is discussed at length by Carroll [Carroll, 1995].

Initial calculations with Blaze II using the added reaction package, listed in Table 2, were performed for our flow tube setup with pure oxygen in the flow system. Using output from GlobalKin, a one-to-one comparison was made between the two codes downstream of the discharge and the results were found to be in close agreement. To properly model the

discharge physics, GlobalKin contains an extensive kinetic package including electrons and various positive and negative ions. It appears that the reduced kinetic package presented in Table 2 is sufficient for modeling the oxygen kinetics outside of the discharge region.

One of the first things observed when the kinetic package of Table 2 was added was the decay of the O₂(¹□) concentration with distance downstream, Fig. 2. Prior calculations with the classic COIL kinetic package did not show this decay. Examination of the added kinetics pointed clearly to reactions 49 and 50 as being critical to this process and zeroing those reactions eliminated the decay, Fig. 3. This is an important observation because it explains the observed experimental decay by King *et al.* [King, 2002] as being attributable to the presence of O atoms in the flow at the exit of the discharge. Another very interesting result of the modeling is that the flow temperature heats up significantly as energy is removed from the O₂(¹□) state

and converted to translational energy in the flow, Fig. 4. When reactions 49 and 50 were zeroed, this temperature rise was small and can probably be attributed to the pooling reaction, reaction 1, or the removal of O_3 via reactions 53 and 54.

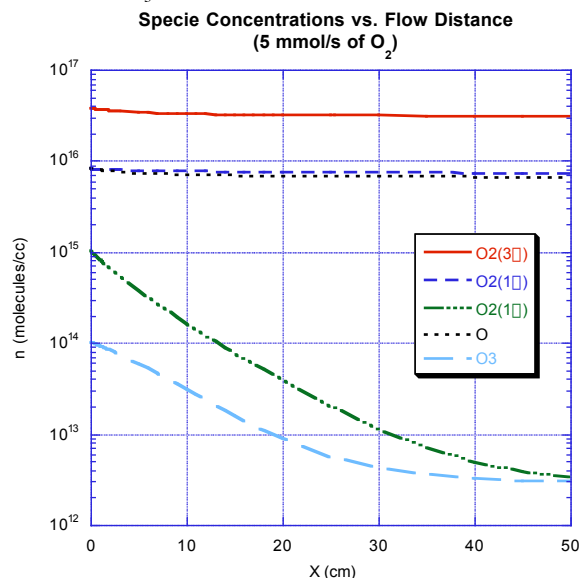


Fig. 2. Oxygen specie concentrations as a function of flow distance for a pure oxygen flow at 5 mmol/s and a pressure of 1.94 Torr.

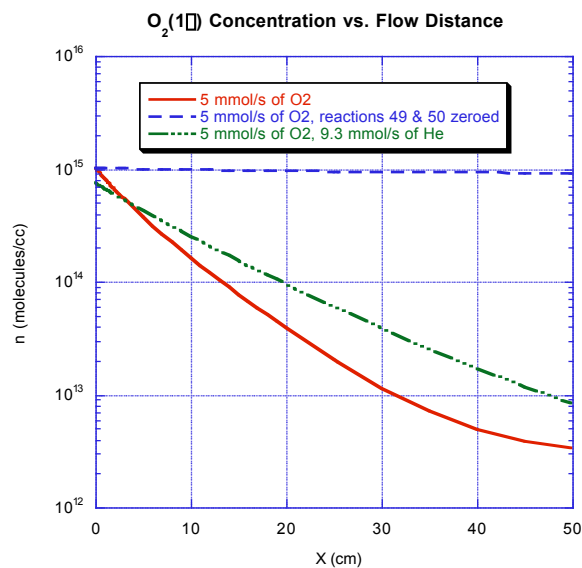


Fig. 3. $O_2(^1\Pi)$ concentration as a function of flow distance for a pure oxygen flow at 5 mmol/s and a pressure of 1.94 Torr. The baseline case is compared with the same case having reactions 49 and 50 zeroed and for a case with He diluent at 3.88 Torr. (Note: the slightly lower initial concentration of O_2 in the case with He diluent is a consequence of having nearly three times the total molar flow rate, but only twice the pressure, a higher velocity and thus lower density of O_2 .)

Another experimental trend that Blaze II matched was that the addition of Helium to the flow reduced the rate of fall of the $O_2(^1\Pi)$ state, Fig. 3, in large part due to the increased flow velocity when Helium was added. Also of significant interest is the fact that the flow temperature rise is significantly lower when there is Helium diluent in the primary flow, Fig. 4. This is a consequence of the higher molar flow rate with helium.

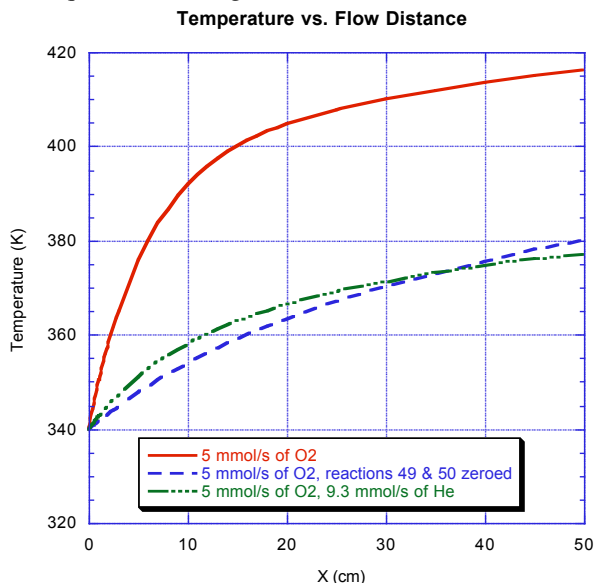


Fig. 4. Temperature as a function of flow distance for a pure oxygen flow at 5 mmol/s and a pressure of 1.94 Torr. The baseline case is compared with the same case having reactions 49 and 50 zeroed and for a case with He diluent at 3.88 Torr.

4.1 Subsonic Studies with Single Iodine Jet

To better understand the kinetics and flow processes with iodine in the flow, a series of Blaze II computations were run for the flow tube setup with a single iodine jet centered in the subsonic flow tube with the injector hole pointed in the primary flow direction, i.e. parallel to the main flow of oxygen. While a supersonic flow system will likely produce a higher efficiency laser, this particular subsonic arrangement is very useful for basic research and is relatively easy to simulate.

The baseline condition modeled is a 5 mmol/s primary flow of O_2 and a secondary stream consisting of 0.025 mmol/s of I_2 and 1 mmol/s of secondary He diluent. Based on measurements by Verdeyen *et al.* [Verdeyen, 2002] and many others, the baseline yield of $O_2(^1\Pi)$ is taken to be 16% and $O_2(^3\Sigma)$ is taken as 2% of the flow. Based upon GlobalKin output and experimental data by Ivanov [Ivanov, 1999], the concentration of O atoms is taken to be the same as $O_2(^1\Pi)$. From GlobalKin output the ozone concentration is taken as 0.2% of the flow. The

pressure of the flow is 1.94 Torr. Thermocouple and spectroscopic temperature measurements of the O₂ flow indicate a temperature of approximately 340 K. The I₂ lines were heated and the secondary flow temperature at the injection point is also assumed to be 340 K. The flow tube has a 1.9" (4.826 cm) I.D. and the iodine injector hole was 3/32" (0.238 cm) in diameter. The initial Mach number of the entire flow (primary plus secondary) for these conditions is 0.097. Note that the Blaze II starting point for Figs 5-14 is at the iodine injection point, which is downstream of the RF discharge.

The predicted gain curve for the baseline case is illustrated in Fig. 5. It is clear that there is only absorption for the baseline conditions. Examining the fluid properties in the simulated flow reveals that the temperature of the mixed flow region is very high, Fig. 6, which is primarily a consequence of the heat release that occurs during the iodine dissociation process.

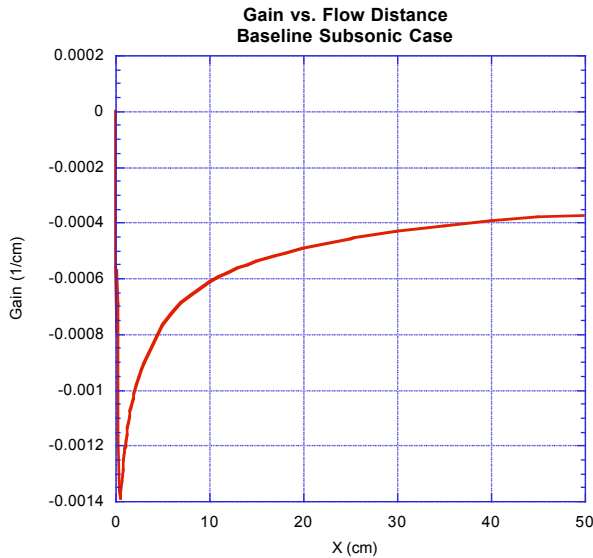


Fig. 5. Gain (absorption) as a function of flow distance for the baseline subsonic mixing case with a single iodine jet.

Temperature is a critical issue because of the equilibrium of the forward and backward rates of the pumping reaction, Eq. (1), [reactions 21 and 22, Table 1]. The threshold yield, Y_{th} , of O₂(¹Δ) required for positive gain as a function of the laser cavity temperature, T_{cav} , can be expressed by [Hon, 1996]

$$Y_{th} = \frac{1}{(1 + 2k_{eq})} = \frac{1}{[1 + 1.5 \exp(401/T_{cav})]} \quad (4)$$

Equation (4) is illustrated graphically in Fig. 7.

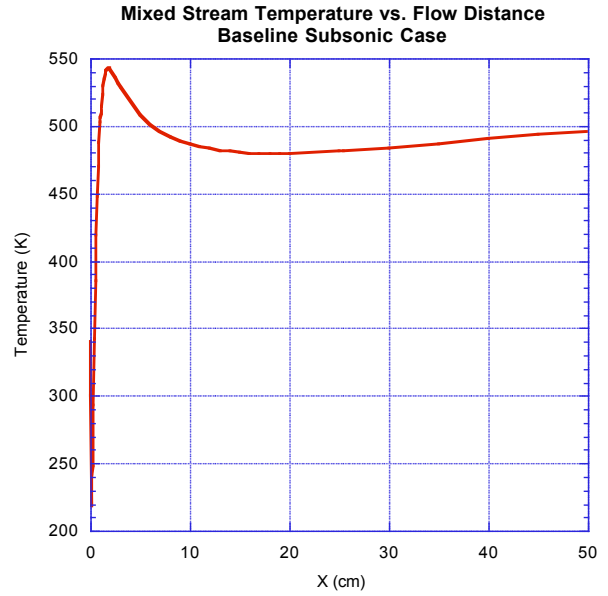


Fig. 6. Mixed stream temperature as a function of flow distance for the baseline subsonic mixing case with a single iodine jet.

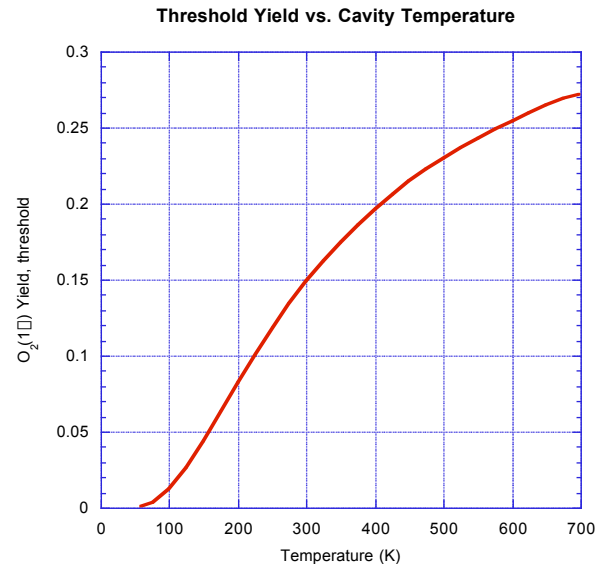


Fig. 7. Threshold yield as a function of laser cavity (mixed stream) temperature for positive gain.

From Fig. 7 it is clear that the baseline case yield of 16% requires that the mixed stream temperature stay below approximately 320 K for positive gain. Figure 6 shows that the mixed flow temperature is reaching approximately 500 K, which from Fig. 7 would require a yield of around 23% for positive gain. Hence, given the predicted temperature rise, it is not surprising that the baseline case exhibits absorption.

The question that arises is, what routes are there for improving the baseline conditions to produce positive

gain from which to perform a lasing demonstration? There are several possible approaches:

- 1) Improve the $O_2(^1\Delta)$ yield from the discharge,
- 2) Pre-cool the primary flow so that the mixed stream temperature will also be lowered,
- 3) Reduce the iodine flow rate to lower the heat released in the I_2 dissociation process,
- 4) Pre-dissociate the iodine molecules prior to injection to eliminate the chemical heat release associated with the I_2 dissociation process,
- 5) Add diluent to absorb chemical heat release and lower the temperature,
- 6) Expand the flow supersonically via a nozzle.

Combinations of these approaches may also be effective in achieving positive gain. It should be noted that pre-dissociating the molecular iodine prior to injection will eliminate the effective yield loss required for dissociation, however, it is still the mixed stream (cavity) temperature that will dictate the minimum yield required to achieve gain above zero.

To examine the first possibility a set of cases were run with increasing yield output from the discharge, Fig. 8. As indicated earlier, it is not surprising that the only one of these calculations producing positive gain was the 25% yield case. There is no question that higher yields from the electric discharge will improve system performance and this will continue to be a key focus of the ongoing experimental program.

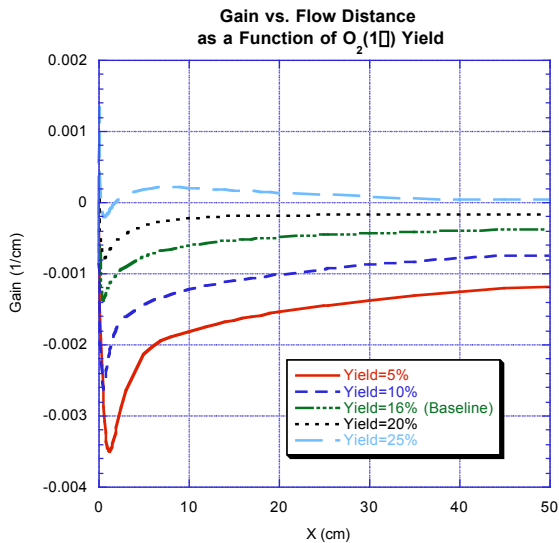


Fig. 8. Gain (absorption) versus flow distance as a function of $O_2(^1\Delta)$ yield for subsonic mixing with a single iodine jet.

A set of calculations was performed for decreasing primary flow temperature, Fig. 9. While this reduced the amount of absorption (increased the gain), it is seen from Fig. 10 that the temperature of the mixed stream is

still too high (above 320 K for a yield of 16%). Note that while the primary oxygen temperature is being reduced for these cases the secondary flow containing the iodine was kept at 340 K. The combination of the hot iodine plus the heat released from the chemical dissociation reactions was enough to keep the temperature too hot despite a primary flow temperature of as low as 140 K. However, the trend indicated by lowering the primary stream temperature is useful and strongly suggests the possibility of lowering the primary temperature in conjunction with another approach.

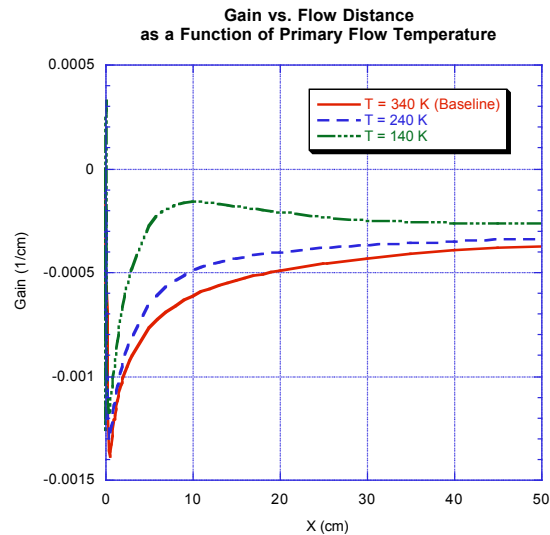


Fig. 9. Gain (absorption) versus flow distance as a function of primary flow temperature for subsonic mixing with a single iodine jet flowing 0.025 mmol/s of I_2 .

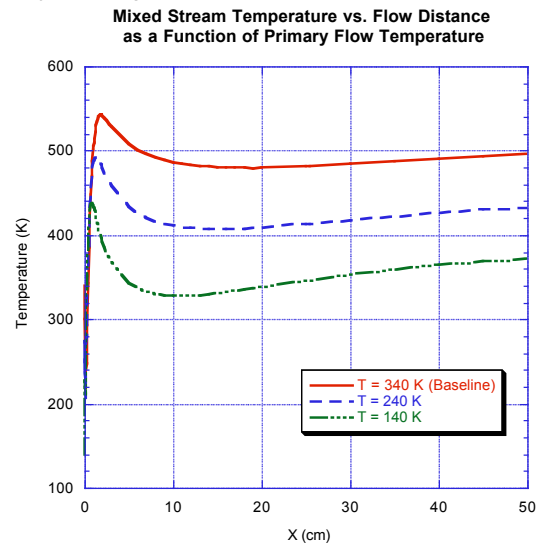


Fig. 10. Mixed stream temperature versus flow distance as a function of primary flow temperature for subsonic mixing with a single iodine jet flowing 0.025 mmol/s of I_2 .

The next series of calculations examined the combined effects of a lower iodine flow rate of 0.010 mmol/s along with lowered primary flow temperatures. Figures 11 and 12 show that positive gain is predicted for the 140 K primary flow temperature case.

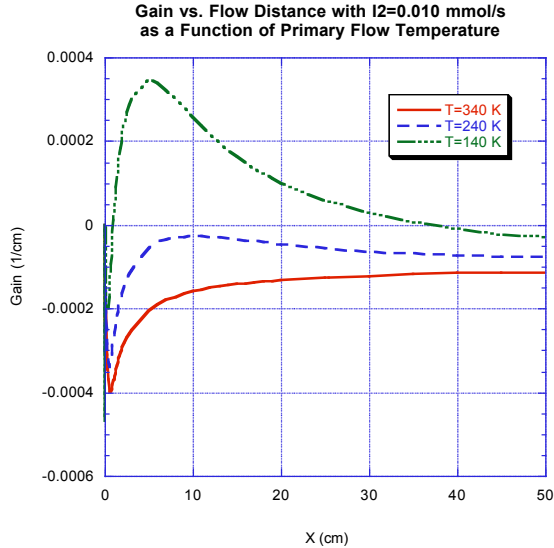


Fig. 11. Gain (absorption) versus flow distance as a function of primary flow temperature for subsonic mixing with a single iodine jet flowing 0.010 mmol/s of I_2 .



Fig. 12. Mixed stream temperature versus flow distance as a function of primary flow temperature for subsonic mixing with a single iodine jet flowing 0.010 mmol/s of I_2 .

Comparing Figs. 11 and 12 with their 0.025 mmol/s of I_2 counterparts, Figs. 9 and 10, shows how the reduced flow rate of I_2 lowers the mixed stream temperatures, and in the 140 K case permits the cavity temperature to

drop below the 300 K point, thereby producing a positive gain system.

Simulations to test the effects of pre-dissociating the molecular iodine prior to injection were studied next. A calculation with the baseline conditions and 100% iodine pre-dissociation showed a reduced absorption and a significantly reduced temperature, but still above 350 K. As such a set of calculations were performed for the nominal 0.025 mmol/s of I_2 , but with a primary flow temperature of 140 K, Figs. 13 and 14.

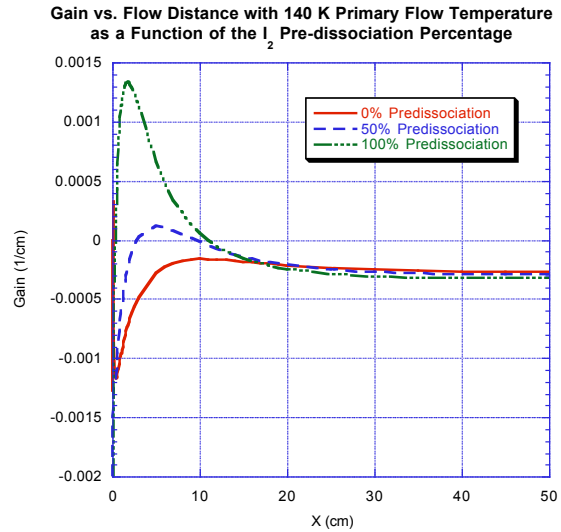


Fig. 13. Gain (absorption) versus flow distance as a function of I_2 pre-dissociation percentage for subsonic mixing with a single iodine jet and primary flow temperature of 140 K.

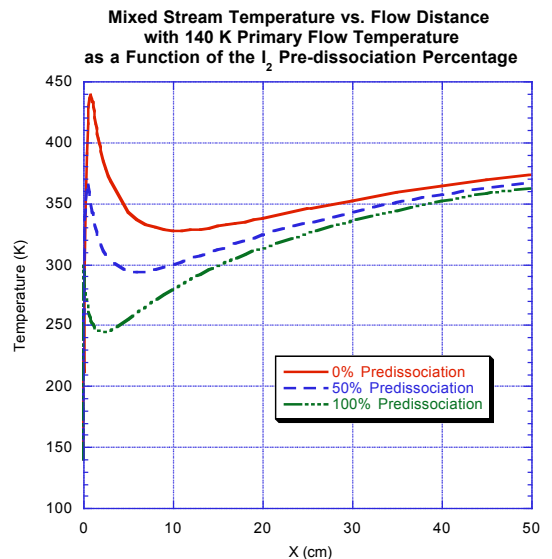


Fig. 14. Mixed stream temperature versus flow distance as a function of I_2 pre-dissociation percentage for subsonic mixing with a single iodine jet and primary flow temperature of 140 K.

Figure 14 illustrates how injection of pre-dissociated iodine substantially drops the initial temperature rise in the mixed stream that occurs from the kinetics associated with dissociating the iodine molecules.

Other cases in the parameter space that were run that produced positive gain were the 0.010 mmol/s of I_2 flow conditions in conjunction with 140 K primary stream flow and both 50% and 100% pre-dissociation. 0.010 mmol/s of I_2 flow in conjunction with 240 K primary stream flow and 100% pre-dissociation also gave positive gain.

5.0 Supersonic Studies

The VertiCOIL [Rittenhouse, 1999; Carroll, 2000] nozzle and typical flow conditions were chosen as the starting point for studies of performance of a supersonic ElectriCOIL system. For these calculations the iodine is injected into the subsonic region of the flow with the nozzle throat located approximately 1.1 cm downstream from the injection point. Initial calculations were performed assuming a 20% yield of $O_2(^1\Sigma)$ and the effect of I_2 pre-dissociation was examined, Fig. 15. Note that these initial supersonic calculations include zero O-atoms and a small 10^{-5} mass fraction of $O_2(^1\Sigma)$, as in classic COIL. The exclusion of O-atoms and any significant fraction of $O_2(^1\Sigma)$ permits us to study the effects of only decreasing the yield of $O_2(^1\Sigma)$. The gain curve for this supersonic cavity with a 20% yield and no pre-dissociation was found to be very low and would not make an efficient laser. However, note that the gain is positive because the temperature of the flow in the laser cavity region drops below 150 K. When the molecular iodine is completely pre-dissociated, then the gain curve, even with a 20% yield, increased to almost 1%/cm, Fig. 15, which compares very favorably with the classic COIL type gain curve.

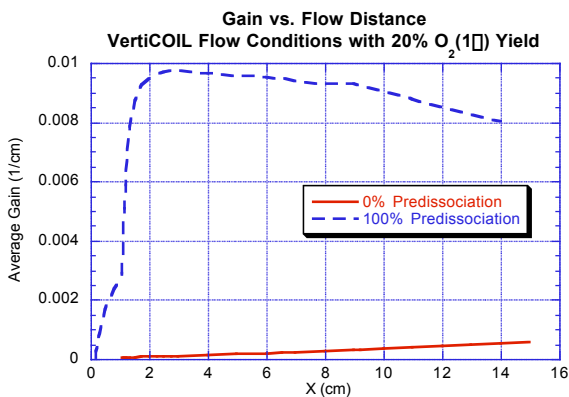


Fig. 15. Gain versus flow distance as a function of I_2 pre-dissociation percentage for supersonic mixing with multiple iodine jets.

A set of simulations was performed varying the yield of $O_2(^1\Sigma)$ to determine the variation of gain in the supersonic case, Fig. 16; 100% iodine pre-dissociation was used for this series of simulations. While absorption is seen upstream of the throat, even the 14% yield case still produces very significant gain levels of approximately 0.8% in the cooled laser cavity.

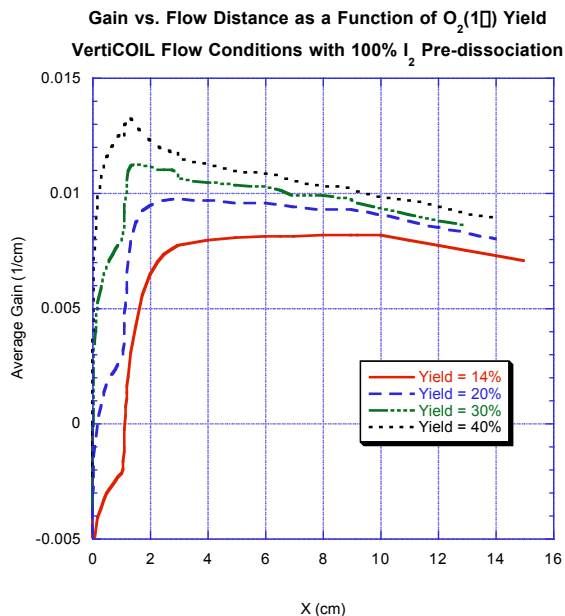


Fig. 16. Gain versus flow distance as a function of yield for supersonic mixing with multiple iodine jets.

Lastly, power calculations using Blaze II for the ElectriCOIL system, Fig. 17, support the conclusions drawn from the heuristic equation [Hon, 1996] presented in Fig. 1.

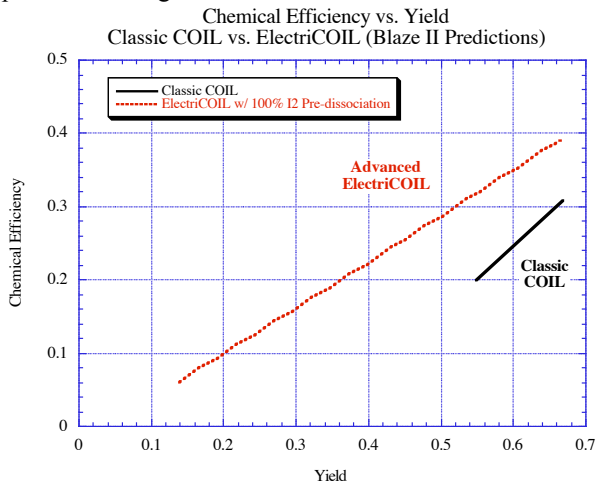


Fig. 17. Chemical efficiency as a function of yield for supersonic mixing with multiple iodine jets.

6.0 Concluding Remarks

A modified kinetic package to more accurately simulate the flow of an ElectriCOIL laser system has been implemented in the Blaze II chemical laser model. The package predicts the decay in the $O_2(^1\Sigma)$ that has been observed experimentally and suggests that the decay is due to reactions between $O_2(^1\Sigma)$ and O atoms. It also predicts that the addition of He diluent reduces the decay rate of $O_2(^1\Sigma)$, also as observed experimentally.

A parametric study established that it should be possible to attain positive gain in the ElectriCOIL system, even with subsonic flow. Temperature proved to be a critical flow variable, especially in the subsonic cases. Two key factors that drive the mixed stream (cavity) flow temperature higher are the chemical kinetics associated with dissociating the iodine molecules, and the deactivation of $O_2(^1\Sigma)$ by O atoms. However, there are several approaches to attaining positive gain:

- 1) Improve the $O_2(^1\Sigma)$ yield from the discharge,
- 2) Pre-cool the primary flow so that the mixed stream temperature will also be lowered,
- 3) Reduce the iodine flow rate to lower the heat released in the I_2 dissociation process, thereby lowering the mixed stream (cavity) temperature,
- 4) Pre-dissociate the iodine molecules prior to injection to eliminate the chemical heat release associated with the I_2 dissociation process,
- 5) Add diluent to absorb chemical heat release and lower the temperature,
- 6) Expand the flow supersonically via a nozzle.

Higher discharge yield and supersonic flow expansion individually are enough to produce positive gain, while combinations of the other approaches 2-4 also result in positive gain. Approach 5, the addition of diluent, needs to be investigated in future simulations.

Simulations of a supersonic ElectriCOIL system indicate that significant performance levels can be attained, even at low yield levels of 20% or less. In addition, pre-dissociation of the iodine is also shown to be very important for the supersonic flow situation. Given the critical nature of the temperature issue, it appears that supersonic flow will be required for the ElectriCOIL system to achieve significant performance levels, but these simulations also indicate that it should be possible to demonstrate a subsonic system.

Acknowledgements

This work was supported by the Air Force Research Laboratory's Directed Energy Directorate SBIR contract F29601-01-C-0007. We would also like to thank B. Woodard for his assistance with laboratory

work, M.J. Kushner for making available and assistance with the GlobalKin model in addition to many helpful discussions, as well as T.J. Madden, G.D. Hager, A. Ionin, and A. Napartovich for many useful consultations on this topic.

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