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Modeling of the chemical generation of atomic iodine in a chemical oxygen-iodine laser

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ABSTRACT

The mathematical modeling of reaction systems for chemical generation of atomic iodine is presented. This process can be applied in the chemical oxygen-iodine laser (COIL), where it can save a substantial part of energy of singlet oxygen and so increase the laser output power. The parametric study of the production of atomic fluorine and subsequently atomic iodine in dependence on the pressure and dilution with inert gas was made. The calculation of the interaction between produced atomic iodine and singlet oxygen was made with four different mixing/reacting schemes.

Keywords: chemical oxygen-iodine laser, atomic iodine, modeling, gas reactions

1. INTRODUCTION

In conventional COIL systems, iodine atoms in the ground state, $I(^2P_{3/2})$, are formed from molecular iodine dissociated by the energy of singlet oxygen, $O_2(^1\Delta_2)$. The using of atomic iodine instantly prepared in other way can substantially increase the chemical efficiency of the laser. Up to now, methods of microwave discharge pre-dissociation of molecular iodine¹, and discharge dissociation of alkyl iodides² were tested to generate atomic iodine for COIL.

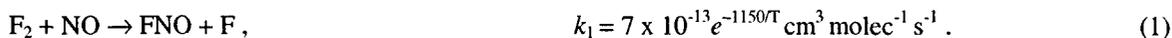
We proposed a method of chemical generation of atomic iodine for COIL based on the reaction of hydrogen iodide with chemically generated atomic fluorine or chlorine.^{3,4} Atomic iodine produced in this way can then undergo the energy transfer from singlet oxygen contained in the gas flow. Because the reaction of hydrogen iodide with both atomic fluorine and chlorine is very fast, the chemical efficiency of atomic iodine production is determined by the efficiency of the preparation of atomic fluorine (in reaction $F_2 + NO$) or chlorine ($ClO_2 + NO$). To estimate the efficiency of these processes, a simplified one-dimensional (1-D) kinetic model was proposed and numerically solved for both reaction systems.⁴ In this modeling, a constant gas velocity and constant total enthalpy were assumed, and the diffusion of species and heat transfer along the flow were neglected. The calculations were performed for the conditions that correspond with the subsonic channel, i.e., upstream the nozzle throat, in the supersonic COIL device operated in our laboratory: the total pressure of 4 kPa, temperature of 300 K, velocity of 200 m/s. The results following from this modeling showed that atomic fluorine is produced with a rate that is too slow to realize this process directly in the subsonic channel. More promising results were obtained by the modeling of the reactions with atomic chlorine, resulting in a sufficient production rate of atomic iodine. However, it is a disadvantage of this process, that the produced atoms are rapidly recombined in the presence of NO_2 . The results of 1-D modelling of this system⁴ are only in some respect in quantitative accordance with the results from the experiments.^{3,5}

The new results of modeling of the production of atomic iodine via atomic fluorine are presented in this paper, including the dependence on the initial pressure and dilution with the inert gas. The results of calculations of the interaction between produced atomic iodine and singlet oxygen are also included, considering four different mixing/reacting schemes.

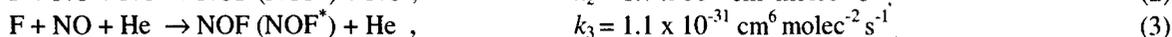
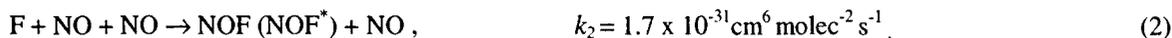
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2. DESCRIPTION OF REACTION MECHANISM

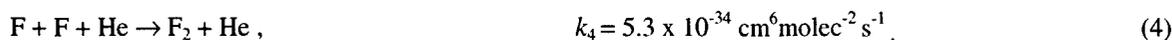
Fluorine atoms are produced by the fast exothermic reaction ($\Delta H^0_{298} = -77$ kJ/mol) of molecular fluorine with nitrogen oxide⁶⁻⁸



The yield of F atoms is substantially influenced by several consecutive reactions, mainly the termolecular reactions of F atoms with NO and other molecules present in the reaction system (e.g., helium used as a diluent)^{9,10}

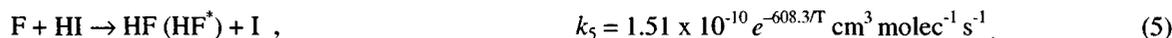


Nitrosyl fluoride, NOF, is formed either in the ground or electronically excited state. The reactions (2) and (3) are also very exothermic (for NOF ground state, $\Delta H^0_{298} = -229.4$ kJ/mol). The three-body recombination of F atoms by the exothermic reaction ($\Delta H^0_{298} = -158.3$ kJ/mol)¹⁰



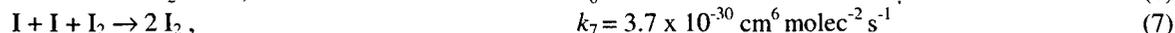
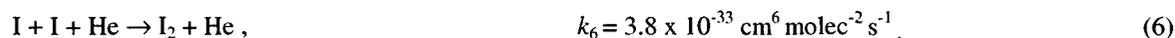
cause another loss of produced fluorine atoms. The 20-30 % efficiency of F atom production in the reaction system including reactions (1)-(4) predicted by Helms *et al.*¹¹, corresponded well with their experimental results. Hoell *et al.*¹² published the calculated F yield of 18 %.

Atomic iodine is generated by the fast reaction ($\Delta H^0_{298} = -261.7$ kJ/mol) of F atoms with hydrogen iodide^{13,14}

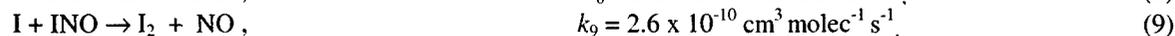
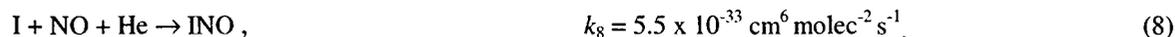


The energy liberated in this process is partly stored in vibrationally excited HF molecules. The contribution of HF* can exceed 56 %, according to Jonathan *et al.*'s study.¹³ The exoergicity of the reaction (5) may suffice even to form electronically excited iodine atoms, $\text{I}(^2\text{P}_{1/2})$ with the branching ratio that was theoretically estimated¹⁵ up to the value of 0.5, however the experimental value obtained by using a high resolution Fourier transform spectrometer¹⁴ did not exceed the value of 0.005.

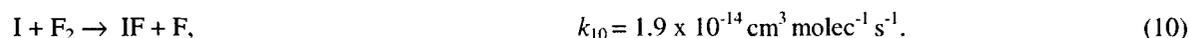
The resultant efficiency of I atom production is influenced (in addition to the above loss-processes of F atoms) by the reactions which consume I atoms, the termolecular recombination of I atoms in the presence of buffer gas (He) and molecular iodine^{16,17}



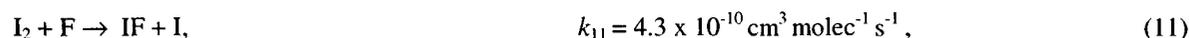
The unreacted nitrogen oxide may cause the loss of I atoms by the mechanism¹⁸



while the reaction of atomic iodine with unreacted fluorine is slow



Molecular iodine produced in the processes (6)-(9) can also react with F atoms to form atomic iodine¹⁷



where IF is formed in both ground and excited states.

3. DESCRIPTION OF MATHEMATICAL MODEL

One-dimensional numerical model used in our previous paper⁴ supposed the constant velocity of gas and consequently constant volume flowrate. However, this assumption is not valid in the case of highly exothermic reactions where temperature significantly rises along the reaction coordinate, the mixture expands and accelerates. The species concentrations are changing not only due to chemical reactions but also due to increase in volume flowrate. In the presented model, the species molar flowrates were calculated according to the differential equation

$$u \frac{d\dot{n}_j}{dx} = \sum_i \frac{k_i}{\dot{V}^{v_k+v_l-1}} \dot{n}_k^{v_k} \dot{n}_l^{v_l}, \quad (12)$$

where $u = \dot{V} / A$ is the gas velocity, x the reaction coordinate, $\dot{n}_j, \dot{n}_k, \dot{n}_l$ are the molar flowrates of species j, k, l , k_i is the rate constant of the i -th reaction, v_k, v_l are the exponents of the kinetic equation and A is the cross-section of the reaction channel.

The volume flowrate \dot{V} was evaluated according to the ideal gas equation of state:

$$\dot{V} = \frac{\sum_j \dot{n}_j RT}{p}. \quad (13)$$

Temperature and pressure changes were calculated by the simultaneous solving of the equation for the total enthalpy conservation

$$\frac{d}{dx} \left(\sum_j \int c_{p,j} dT + \frac{1}{2} \rho_m u^2 \right) = \sum_j \left(-h_j^0 + \int c_{p,j} dT \right) \frac{d\dot{n}_j}{dx}, \quad (14)$$

where $c_{p,j}$ and h_j^0 are the molar heat capacity and enthalpy of formation of species j and ρ_m is the molar density of mixture, and the dynamic equation

$$dp + M \rho_m u du = 0 \quad (15)$$

where M is the molar weight of the mixture.

This set of equations was numerically solved using the fourth-order Runge-Kutta routine.

4. MODELING OF F AND I ATOMS PRODUCTION. RESULTS AND DISCUSSION.

4.1 Production of F atoms

The production of F atoms was modeled including the reactions (1)-(4) for several values of initial pressure, helium dilution and initial concentration ratio [NO]:[F₂]. The results are summarized in Tab. 1. It is obvious, that the conversion of F₂ molecules to F atoms rapidly decreases and the reaction path becomes shorter with increasing of the initial pressure. The conversion substantially declines with increasing the ratio of rates of reactions (2), (3) and (1):

$$\frac{r_2 + r_3}{r_1} = \frac{k_2 [F][NO]^2 + k_3 [F][NO][He]}{k_1 [F_2][NO]}. \quad (16)$$

Tab. 1. Production of F atoms. $\eta_F = n(F)_{max}/n(F_2)_0$ is the maximum conversion of F_2 to F, T , p , and τ are values of temperature, pressure and reaction time calculated at the place of maximum conversion.

[NO]:[F ₂]	p ₀ (kPa)	[He]:[F ₂]	η_F	T (K)	p (kPa)	τ (ms)
2	1	23	0.70	490.6	1.44	4.0
2	2	23	0.50	514.3	2.55	1.7
2	4	18	0.41	586.7	4.64	0.6
1	4	23	0.34	517.8	4.43	3.2
2	4	23	0.35	536.6	4.48	0.7
2	4	41	0.24	442.4	4.23	1.3
2	10	23	0.20	564.9	10.27	0.2

This ratio becomes higher with increasing both, the pressure and helium dilution. The conversion is not influenced by the initial ratio [NO]:[F₂], but significant amount of NO remains unreacted at [NO]:[F₂] > 1. The effect of residual content of F₂ or NO on the I* quenching is discussed in Sec. 5.

The expression (16) depends also on the temperature. The constants k_2 , k_3 are taken as temperature independent, but k_1 increases with temperature (eq.(1)). Consequently, as the mixture temperature rises due to the exothermic reactions, the production rate of F atoms increases too. The calculated increase in temperature ($\Delta T = 140 - 260 K$) probably results also in the increase of the rates of reactions (2) and (3). The temperature dependence of these reactions was not measured, but is supposed to be relatively small.⁹

The concentration profiles for the conditions typical for the subsonic part of the COIL (4 kPa) are shown in Fig. 1.

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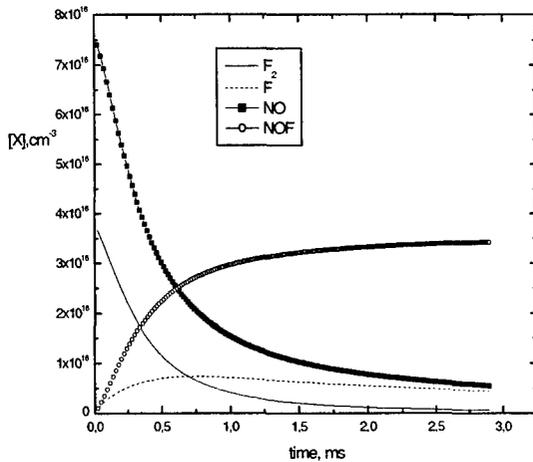


Fig. 1. Fluorine atoms production. Time development of concentrations of different species. Initial concentration ratio [F₂]:[NO]:[He]=1:2:23, initial pressure 4 kPa, initial temperature 300 K.

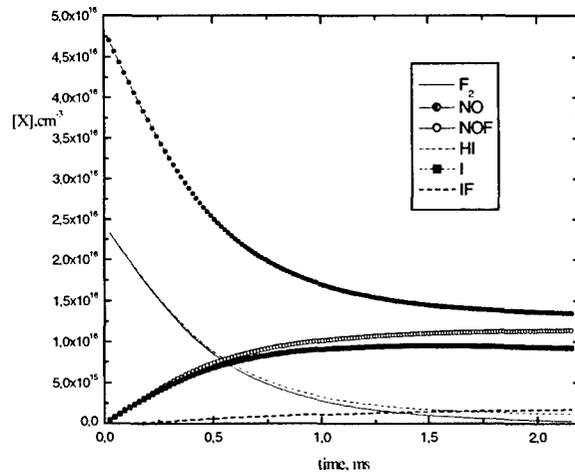


Fig. 2. Iodine atoms production. Time development of concentrations of different species. Initial concentration ratio [F₂]:[NO]:[HI]:[He]=1:2:1:36, initial pressure 4 kPa, initial temperature 300 K.

The conversion does not overcome 35 %. In accordance with the previous modeling⁴, it can be concluded that the production of F atoms is too slow under these conditions. Then, assuming the gas velocity of 200 m/s, HI will have to be introduced into the flow channel at the 20 cm distance from the F₂/NO injection.

The other possibility is to produce F atoms in a separate reactor and then to introduce them together with HI into the O₂(¹Δ_g) flow, as described in Sec. 5.1.

4.2 Production of atomic iodine

In recent modeling⁴ it was found, that simultaneous admixing of F₂, NO, and HI can give promising results in atomic iodine production efficiency. In this case, hydrogen iodide reacts instantly with formed F atoms, and reduces the rate of the loss reactions (2) and (3). This process was modeled including the reactions (1) - (11) under the assumptions described in Sec. 3. The results are summarized in Tab. 2.

Tab. 2. Production of I atoms. $\eta_I = n(I)_{max}/n(F_2)_0$ is the maximum conversion of F₂ to I, T , p , and τ are values of temperature, pressure and reaction time calculated at the place of maximum conversion.

[NO]:[F ₂]	p ₀ (kPa)	[He]:[F ₂]	η_I	T (K)	p (kPa)	τ (ms)
2	1	9	0.86	1373	1.00	5.5
2	1	18	0.88	976	1.00	5.8
2	1	36	0.89	692	1.00	9.9
1	1	37	0.68	611	1.00	10
2	4	36	0.84	652	4.57	1.5
2	10	36	0.64	642	10.0	0.5

The effect of helium dilution on the conversion of F₂ to I atoms is very small on the contrary to the F atoms production. The conversion is higher by 20% at the initial concentration ratio [NO]:[F₂]=2:1 against 1:1. The time course of concentrations for the initial pressure of 4 kPa is shown in Fig. 2. It can be seen that the reaction time for reaching the maximum conversion is approximately two times longer in comparison with F atom generation. It could be ascribed to the additional process producing I atoms in reaction (11).

The degree of the conversion of F₂ to F atoms (in the system F₂+NO), and F₂ to I atoms (in the system F₂+NO+HI) in dependence on the initial pressure is shown in Fig. 3. It follows from the comparison of the two dependencies that the conversion to F atoms rapidly decreases with increasing pressure, while the conversion to I atoms is less pressure dependent. This is caused by the suppression of the loss reactions (2) and (3), so the ratio (16) is much less pressure dependent.

The calculated increase in temperature for both, the F and I atoms production is independent on the initial pressure. The heating of the mixture is, of course, dependent on the dilution by helium. The temperature does not exceed 550 K in the case of F atoms production and 700 K in the case of I atoms production, if there is a sufficient dilution with inert gas (the dilution ratio [F₂]:[He] = 1:30 corresponds to the amount of helium contained in the COIL primary gas).

It should be noted, that the calculations included only particles in the ground electronic state. The excited particles NOF*, HF*, and IF* are also formed and hence the reaction enthalpy is partly transformed to the excitation energy. The resulting reaction temperature should be therefore lower than the values presented in Tables 1 and 2.

The results of the modeling of F and I atoms production were used in calculations of the I* production when produced atoms were introduced into the stream of singlet delta oxygen.

5. MODELING OF I* PRODUCTION

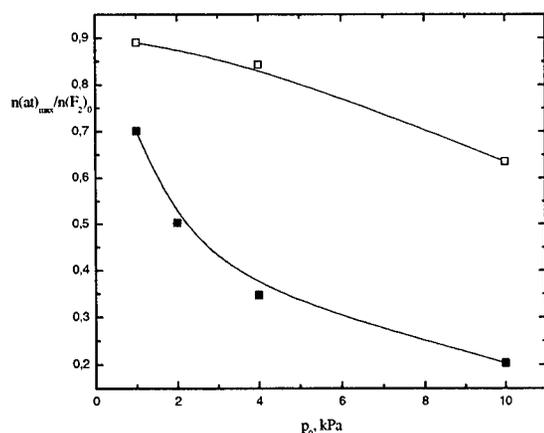


Fig. 3. Conversion of F_2 to F atoms in the mixture of F_2 and NO (solid symbols) and conversion of F_2 to I atoms in the mixture of F_2 , NO and HI (open symbols) in dependence on the initial pressure. Helium dilution $[F_2]:[He] = 1:30$.

supersonic mixing assumes the pressure of 0.5 kPa and temperature of 200 K. The results of F/I atoms production at 10 kPa are used in the case of subsonic mixing and results for F/I atoms production at 1 kPa in the case of supersonic mixing (see Fig. 4).

The constant temperature was assumed in this modelling, with aim to save the computer time.

The initial concentration ratio of F or I atoms and $O_2(^1\Delta_g)$ was chosen according to the known optimal ratio $[I_2]/[O_2] = 1:50$ for COIL operation, i.e.:

$$\frac{[I]_0}{[O_2(^1\Delta)]_0} = \frac{2}{50 - N}, \quad (17)$$

where N is the number of molecules of $O_2(^1\Delta_g)$ consumed for the dissociation of one I_2 molecule. In the following calculation, the value $N=5$ was assumed.

5.2. Results and discussion

5.2.1 F + HI + $O_2(^1\Delta_g)$ system

Time development of the concentration of iodine $I(^2P_{1/2})$ state at the subsonic conditions is shown in Fig. 5 (solid line). The concentration rises up to 0.13 ms and then slowly decreases. Assuming the average gas velocity of 200 m/s, the maximum concentration is attained at a distance of 2.6 cm. Under the supersonic conditions, the excitation rate is very low (see Fig. 6, solid line). If the supersonic gas velocity of 1000 m/s is assumed, the maximum concentration is attained at the distance of 1 m.

5.1 Description of reaction conditions

The 1-D modeling of reactions between primary and secondary gases in COIL can describe the real three-dimensional process only approximately and must include some additional terms which make the correction on the limited rate of gases mixing.^{19, 20} Nevertheless, for the first estimation of this process they can be neglected. Our aim is to compare the suggested mixing schemes from the kinetic point of view with a special interest on the lifetime of I^* atoms. The reactions between F, HI and $O_2(^1\Delta_g)$ in the first series and between I and $O_2(^1\Delta_g)$ in the second series are modelled. The calculations start from the results of F or I atoms production process including all reactants and products occurred in the reactions (1)-(11) (secondary gas). The initial values for the primary gas are taken from the typical composition of the gas exiting the singlet oxygen generator, i.e.:

$[O_2]:[He] = 1:2$, $[O_2(^1\Delta_g)]:[O_2(^3\Sigma_g)] = 3:2$ and 3 % of H_2O . The reactions between $O_2(^1\Delta_g)$ and I, I_2 are taken from the reference.²¹

The subsonic mixing conditions include the initial pressure of 4 kPa and temperature of 300 K and the

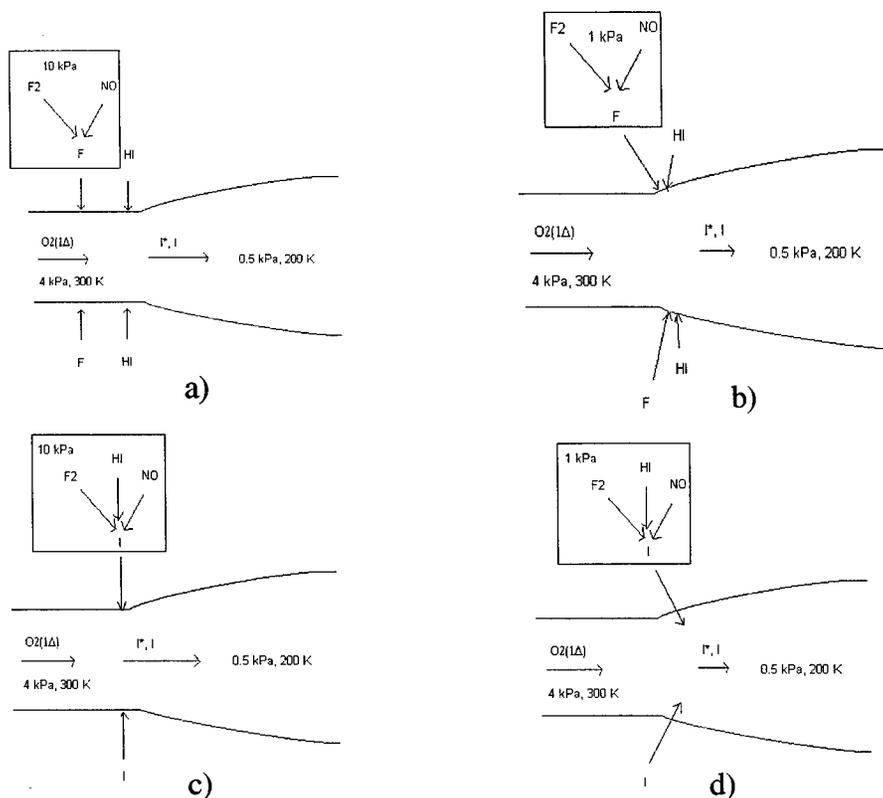


Fig. 4.: Different mixing schemes for I^* generation: a) the subsonic mixing of F, HI and $O_2(^1\Delta_g)$, b) the supersonic mixing of F, HI and $O_2(^1\Delta_g)$, c) the subsonic mixing of I and $O_2(^1\Delta_g)$, d) the supersonic mixing of I and $O_2(^1\Delta_g)$

5.2.2 $I + O_2(^1\Delta_g)$ system

Time development of the concentration of iodine $I(^2P_{1/2})$ state at the subsonic conditions is shown in the Fig. 5 (dashed line). The concentration rises up to 0.04 ms and then rapidly falls. Assuming the average gas velocity of 200 m/s, the maximum concentration is attained at a distance of 8 mm. If the mixing delay is taken into account, the loss of excited iodine in the subsonic channel should not be serious if the injection is placed right before the nozzle throat.

Under the supersonic conditions, the concentration rapidly rises and attains its maximum value before 0.03 ms, which corresponds to a distance of 3 cm (see Fig. 6, dashed line). Then the concentration slowly decreases: for example, 80 % of the maximum value is attained at a distance of 38 cm.

The calculations of the two above mentioned methods were performed with the same initial concentrations of atoms introduced into the flow channel, F atoms in the first method and I atoms in the second one. However, the energy transfer from singlet oxygen to atomic iodine is faster than the reaction (5). That is why the maximum concentration of $I(^2P_{1/2})$ is higher in the case of $I + O_2(^1\Delta_g)$ system and, on the other hand, its subsequent decrease is faster.

The described process of the production of I atoms brings many new species into the laser mixture, that can quench produced excited atomic iodine and singlet oxygen as well. According to the known values of rate constants for quenching of singlet delta oxygen⁴, the influence of the components coming from atomic iodine production is very small.

The known rate constants for quenching of $I(^2P_{1/2})$ are summarized in Tab. 3 (for references, see⁴). The comparison of the quenching by different species calculated from the initial concentrations of reactants provides an interesting insight into the $I(^2P_{1/2})$ lifetime. The initial rates divided by initial I^* concentration for $I + O_2(^1\Delta_g)$ system under subsonic and

Tab. 3. Quenching of $I(^2P_{1/2})$ by components present in the reaction system for I atoms generation

NO	5×10^{-17}
HI	5×10^{-14}
HF	3×10^{-12}
H ₂ O	2.3×10^{-12}
I ₂	3.5×10^{-11}
F ₂	5.0×10^{-14}
O ₂ (¹ Δ _g)	1.1×10^{-13}
IF	1.3×10^{-11}

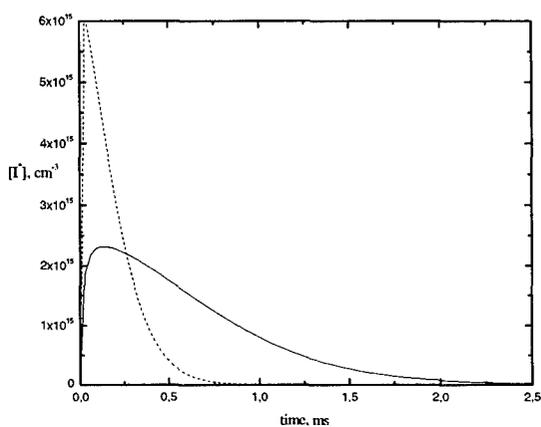


Fig. 5. Concentration profiles of excited iodine for subsonic conditions. Mixing of F, HI and O₂(¹Δ_g) (—), mixing of I and O₂(¹Δ_g) (·····).

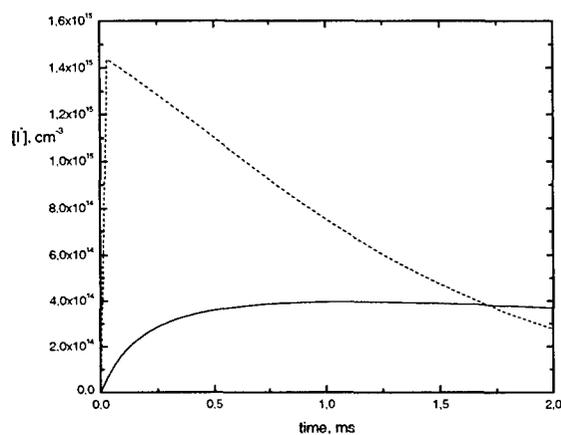


Fig. 6.: Concentration profiles of excited iodine for supersonic conditions. Mixing of F, HI and O₂(¹Δ_g) (—), mixing of I and O₂(¹Δ_g) (·····).

supersonic conditions are shown in Fig. 7a,b. The most effective quenchers are IF and HF molecules. Their quenching effect is two/three times higher than the effect of H₂O molecule that is the well-known serious quencher in COIL medium.²² It must be noted, that the above-mentioned values are valid under the assumption of ground electronic state of IF and HF produced. As mentioned in Sec. 3, these particles are formed partly in the excited state, but the rate constants of $I(^2P_{1/2})$ quenching by IF* and HF* were not published. Ground and excited NOF molecule could be also a serious quencher of $I(^2P_{1/2})$, but the appropriate quenching constant is not known as well. The quenching effect of NO and F₂ is small, so that the residual content of these species should not bring any complications.

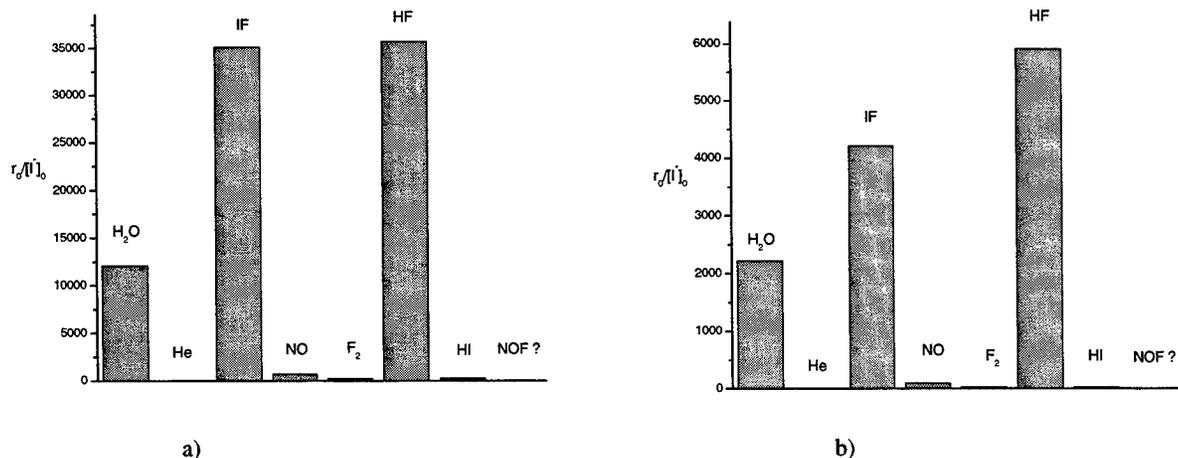


Fig. 7a,b. I* quenching by different molecules. a) subsonic mixing of I and $O_2(^1\Delta_g)$,
b) supersonic mixing of I and $O_2(^1\Delta_g)$

5. CONCLUSIONS

The detailed 1-D mathematical modeling of the chemical production of atomic fluorine and atomic iodine, subsequently, was made. The dependencies of the conversion of F_2 to F or I atoms on the initial pressure and concentration ratios were calculated. It was confirmed that the reaction path for F or I atoms production is too long to be realised directly in the subsonic laser part. In the newly suggested process, F or I atoms are produced in a separate reactor and they are introduced into the stream of $O_2(^1\Delta_g)$. The four different mixing/reacting schemes for reaction between F, HI and $O_2(^1\Delta_g)$ in one case and I and $O_2(^1\Delta_g)$ in the second case were modeled. The supersonic mixing of I and $O_2(^1\Delta_g)$ seems to be the most advantageous process, where atomic iodine is produced separately with good efficiency and the energy transfer from $O_2(^1\Delta_g)$ to atomic iodine is fast at the beginning of the supersonic nozzle. The other possible processes are the subsonic mixing of F, HI and $O_2(^1\Delta_g)$ or I and $O_2(^1\Delta_g)$. The supersonic mixing of F, HI and $O_2(^1\Delta_g)$ gives an insufficient rate of I* production.

ACKNOWLEDGEMENTS

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