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COLLISIONAL – RADIATIVE MODEL FOR CO AND C_2

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In plasmas, when the existence of the local thermodynamical equilibrium is questionable, state-to-state collisional radiative models are required to calculate reliable electron number density and population densities of heavy particles in excited states. By this way, it becomes possible to quantify the exchanges between the numerous energies stored in the inner modes and, for instance, to predict the radiative and collisional contributions to the wall damaging in the case of atmospheric re-entry [1]. In the present study, numerical modeling is used to investigate a pure CO_2 plasma in the frame of studies devoted to the behavior of probes entering Martian atmosphere. The dissociation of CO_2 and the ensuing exchange reactions lead to the formation of CO and C_2. Owing to the strong contribution of these molecules to the energy storage and to the radiative signature of the plasma, it is necessary to estimate accurately the population of their excited states. In the present CR model, the main partners are CO_2, CO, O_2, C_2, C and O and the temperatures are limited to values lower than 10 000K in the purpose of comparing numerical results to the ones derived from spectroscopic measurements currently performed in plasma wind tunnels of CORIA and VKI. The atomic species are assumed to be in their ground state. The designation and energy data of the involved CO and C_2 excited states are displayed in Table I.

The time evolutions of the excited state populations result from the following elementary processes:

(1) **collisional**: besides the classical reactions whose rate coefficients are well-known, it is necessary to take into account of two exchange reactions for determining the CO(i) and C_2(j) densities:

$$C + O_2 \rightarrow CO(i) + O \quad \text{and} \quad C_2(j) + O \rightarrow CO(i) + C$$

We have calculated the rate coefficients of these reactions by developing a simplified approach based on the activated complex theory [2]. Concerning the metastable CO($a^3\Pi$) state, its transport kinetics is simply described by introducing a characteristic diffusion length Λ_0.

(2) **radiative**: the main radiative systems of CO and C_2 have been taken into account in the calculations.

All the elementary processes are put together into the balance equation of the species X in its excited state in the form [3]:

$$\frac{d[X(i)]}{dt} = -v\frac{[X(i)]}{R} - \frac{1}{\Lambda_0^2}\overline{D}_{X(i)}[X(i)] + \left[\frac{\partial[X(i)]}{\partial t}\right]_{Coll,Rad} \qquad (1)$$

where v is the plasma velocity, R its characteristic size and $\overline{D}_{X(i)}$ the X(i) diffusion coefficient.

TABLE 1. Designation and energy data of the excited states involved in the present model[1].

State	g_e	T_e	ω_e	State	g_e	T_e	ω_e
$CO(X^1\Sigma^+)$	1	0.000	0.2690	$C_2(X^1\Sigma_g^+)$	1	0.000	0.2300
$CO(a^3\Pi)$	6	6.036	0.2162	$C_2(a^3\Pi_u)$	6	0.089	0.2035
$CO(a'^3\Sigma^+)$	3	6.921	0.1523	$C_2(b^3\Sigma^-)$	3	0.798	0.1823
$CO(d^3\Delta_i)$	6	7.578	0.1453	$C_2(A^1\Pi_u)$	2	1.040	0.1994
$CO(e^3\Sigma^-)$	3	7.964	0.1386	$C_2(c^3\Sigma_u^+)$	3	1.650	0.2432
$CO(A^1\Pi)$	2	8.068	0.1882	$C_2(d^3\Pi_g)$	6	2.482	0.2217
$CO(D^1\Delta^-)$	2	8.174	0.1356	$C_2(C^1\Pi_g)$	2	4.248	0.2243
$CO(b^3\Sigma^+)$	3	10.392	0.2727	$C_2(e^3\Pi_g)$	6	5.058	0.1372
$CO(B^1\Sigma^+)$	1	10.780	0.2619	$C_2(D^1\Sigma_u^+)$	1	5.361	0.2268

This theoretical approach is therefore purely temporal. For instance, the relaxation of the excitation temperature from a non-equilibrium initial state is displayed in Fig. 1. Our CR model is also able to take possible vibrational non-equilibrium into account. During this conference, we will illustrate the time evolution of the CO_2 plasma under these conditions.

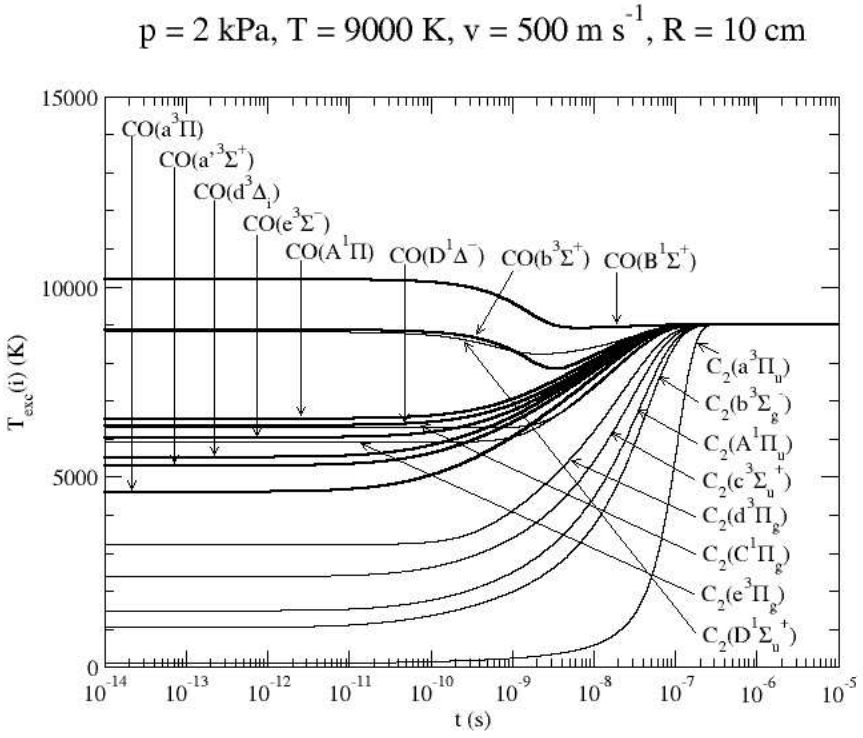

Fig. 1: Excited states relaxation for CO and C_2 calculated by our CR model.

Reference

[1] J.D. Anderson, Jr., 1989 *Hypersonic and high temperature gas dynamics* (McGraw-Hill, NY)
[2] A. Bultel *et al.,* 2010 to be submitted to *Chemical Physics*
[3] A. Bultel *et al.,* 2004 *Physics Letters A* **323** 267

[1] g_e : electronic degeneracy, T_e, ω_e: usual spectroscopic constants (in eV).