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A 2D Model of a Gliding Arc Discharge for CO_2 Conversion

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Abstract. The study presents a 2D fluid plasma model of a gliding arc discharge for dissociation of CO_2 which allows its subsequent conversion into value-added chemicals. The model is based on the balance equations of charged and neutral particles, the electron energy balance equation, the gas thermal balance equation and the current continuity equation. By choosing the modeling domain to be the plane perpendicular to the arc current, the numerical calculations are significantly simplified. Thus, the model allows us to explore the influence of the gas instabilities (turbulences) on the energy efficiency of CO_2 conversion. This paper presents results for plasma parameters at different values of the effective turbulent thermal conductivity leading to enhanced energy transport.

INTRODUCTION

The gliding arc discharge (GAD) is one of the most attractive plasma sources for CO_2 dissociation [1–4]. The topic is extremely up to date due to the global warming and its associated consequences. The main efforts of the optimization of this type of plasma sources are aimed at increasing the conversion and energy efficiency [2–5]. The numerical modeling makes a significant contribution in this direction.

Because of the complicated kinetic of CO_2 and the need of significant computational resources, the models of GAD with detailed plasma chemistry are only few [4–7]. Valuable conclusions follow even from the 0-dimensional model in [4]. It is well known that the CO_2 dissociation is significant when the highly excited vibrational levels of the asymmetric mode are populated. Selection of conditions to maintain appropriate form of the vibrational distribution function is a way to increase the conversion. The model predicts that the gas temperature close to 1000 K and greater power density improve the conversion and energy efficiency. The other important option for optimization is to remove the O atoms from the systems by chemical trapping with H atoms. This would prevent CO and O dissociated particles from recovering to CO_2 through the reverse reaction. One of the disadvantages of the GAD is that the fraction of the treated gas is limited. The 1D model in Ref. [6] shows that only at the distance less than 0.5 mm from the center of the arc the CO_2 dissociation is significant. It is clear that another way to improve the CO_2 conversion would be to enhance the fraction of the gas which can be treated by the arc. A 2D model of Wang et. al. [5] demonstrates the potential of two ways to increase the volume of the treated gas. One of them is to increase the gas velocity and hence the relative velocity of the arc to the gas (in experiments it was observed that the arc gliding velocity can be slightly lower than the gas velocity). This difference affects not only the amount of gas being treated but also its cooling. Other possibility is to use natural phenomena observed at larger gas flow, which are known as "back-breakdown events". As a result a new discharge channel is formed. Increasing the number of this phenomena the conversion of CO_2 and energy-efficiency are improved.

The study presented here is a 2D fluid plasma model which is in scope of the numerical investigation of the GAD [1–7]. The purpose of the simulations is to investigate the impact of gas velocity and turbulence on the energy efficiency of CO_2 dissociation of the discharge. The modeling domain is in plane perpendicular to the arc current, which means that we neglect effects related with the arc extension in the other, non-simulated direction. The latter approximation is reasonable when the particle and energy transport processes are negligible compared to the

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processes in direction transverse to the arc current like for example when the turbulent heat transport is dominant. This configuration can give the possibility for flexible changes of many parameters. In this paper the influence of the turbulence on plasma properties are investigated. The results for energy-efficiency of CO_2 are obtained at different values of turbulent thermal conductivity.

DESCRIPTION OF THE MODEL

The 2D fluid plasma model presented here is structured as the model in Ref. [8]. The set of equations includes the balance equations of charged and neutral particles, the electron energy balance equation, the gas thermal balance equation and the current continuity equation. The quasineutral modeling approach is used [8] and the ambipolar electric field is not included in the particle fluxes in an apparent form. The modeling domain is a cross section of the arc channel, i.e. the plane perpendicular of the arc current. Because of the symmetry only the half part of cross section is modeled.

The CO_2 chemistry is taken into account as in Ref. [6]. The particles in the model are the neutral ground species (CO_2, CO, C, O_2, O), the charged species (CO_2^+, O_2^+, CO_3^-, O_2^-, O^-, e^-) and the neutral excited species ($CO_2(v_a)$, $CO_2(v_b)$, $CO_2(v_c)$, $CO_2(v_d)$, $CO_2(v_1-v_7)$, $CO_2(v_8-v_{14})$, $CO_2(v_{15}-v_{21})$, $CO_2(e_1)$). All symmetric mode vibrational levels $CO_2(v_a, v_b, v_c, v_d)$ are considered separately, while asymmetric mode vibrational levels $CO_2(v_1-v_{21})$, are lumped of 3 groups. It has been observed that this simplification does not have a significant impact on the vibrational distribution function [6].

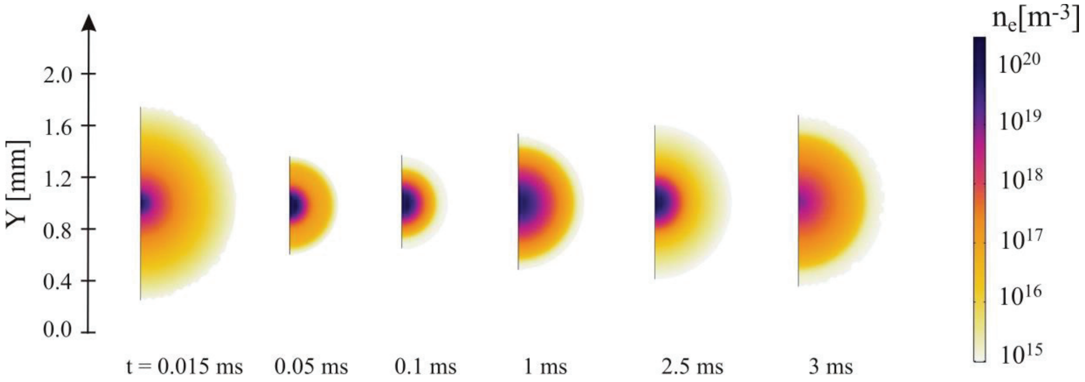


FIGURE 1. 2D plots of the electron density at different moments of time for $k_t = 0$. The cutout range is selected to show a density distribution of $n_e > 10^{15}$ m^{-3}.

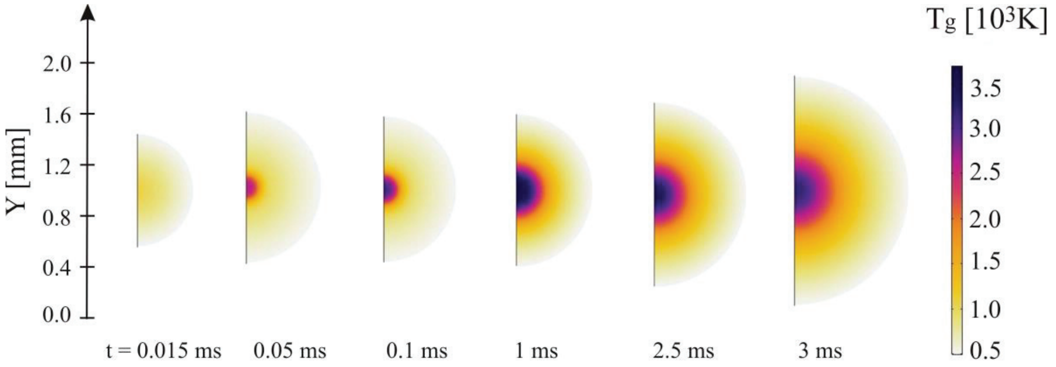


FIGURE 2. 2D plots of the gas temperature at different moments of time for $k_t = 0$. The cutout range is selected to show a gas temperature distribution of $T_g > 500$ K.

The simulation of the arc is started by introducing a heating term for a short time (about 15 μs) in the electron energy balance equation. The heating term is represented by a 2D Gaussian function, with narrow standard deviation

(3×10^{-4} m). From this moment the arc is sustained by external power source with fixed arc current. In time, the electron density increases with two orders of magnitude (Fig. 1). In the model the external power source is switched off at time 2.5ms, and then the arc extinguishes gradually. The value is selected to correspond approximately to a speed of the arc $v_{arc} = 20$ m/s and moving path of 5 cm. In the model the relative velocity of the arc with respect to the gas is not considered.

In this work the DC gliding arc discharge are considered. The current that is achieved in the plasma channel is 20 mA at fixed voltage of 6000 V and a ballast resistor with value 300 kΩ.

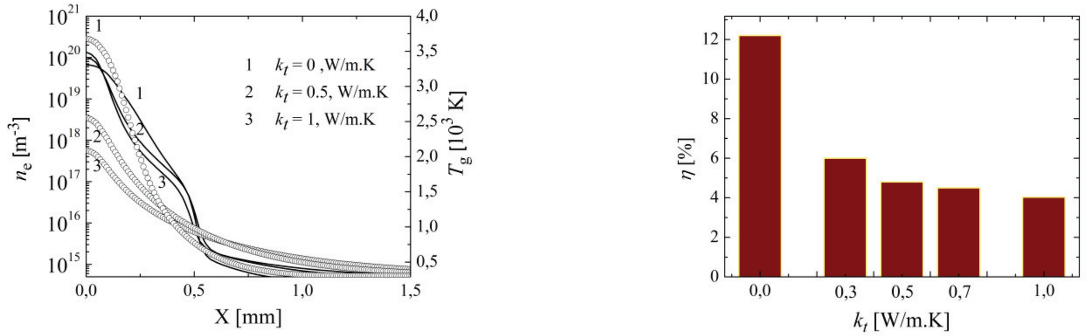
The energy efficiency η of the dissociation of CO_2 is the most informative specification for the application. It is determined by the ratio of the dissociation enthalpy (ΔH = 2.9 eV/molecule) to the actual energy cost of one CO molecule (E_n) produced in a plasma system [1] i.e. $\eta,\% = (\Delta H / E_n)\times 100$.

The effect of the turbulence on η has been investigated in the present work. The different degrees of the turbulence are introduced by the parameter k_t which is an effective thermal conductivity due to turbulent transport, which is added to the gas own molecular thermal conductivity. The values of k_t studied are in the interval from 0 to 1 W/m.K. They are chosen after the simulation based on the Shear Stress Transport Reynolds Averaged Navier-Stokes turbulent model [9] of the gas.

RESULTS AND DISCUSSION

The evolution of the gliding arc is shown in Fig. 1 and 2, with 2D distributions of the electron density (n_e) and the gas temperature (T_g) respectively. At the moment of contraction of the plasma channel (around t = 0.05 ms), the density becomes in the order of 10^{20} m^{-3}. After the arc switch-off time (t = 2.5 ms) the maximum of the plasma density decreases rapidly. The gas heating is shifted over time and the gas temperature reaches a maximum of 3680 K around t = 1 ms (Fig. 3(a)).

The high gas temperatures around 3000 K even after the arc decay time indicates that the cooling of the gas is slow. This values of the T_g is in the range investigated in [4] with significant CO_2 conversion but with reduced energy efficiency. In this condition the energy inserted in the plasma is not primarily used for dissociation. The energy efficiency without turbulence (k_t = 0) from our simulation are comparatively low 12.06% (Fig. 3 (b)). By introducing a turbulent thermal conductivity, the energy efficiency is significantly reduced, for $k_t > 0.5$ it is about 4%. This behavior can be explained with $\eta(T_g)$ dependence (a curve similar to the inverted parabola) obtained in [4]. The presence of turbulence leads to faster cooling (Fig. 3(a)), the gas temperature decrease from 3680 K (k_t = 0) to 2000 K (k_t = 1) at the moment t = 1 ms. The temperature values obtained from the model are in the minimum of the $\eta(T_g)$ curve. In order to achieve optimal conditions for CO_2 dissociation – high energy efficiency and conversion – it is necessary to introduce additional cooling mechanisms.

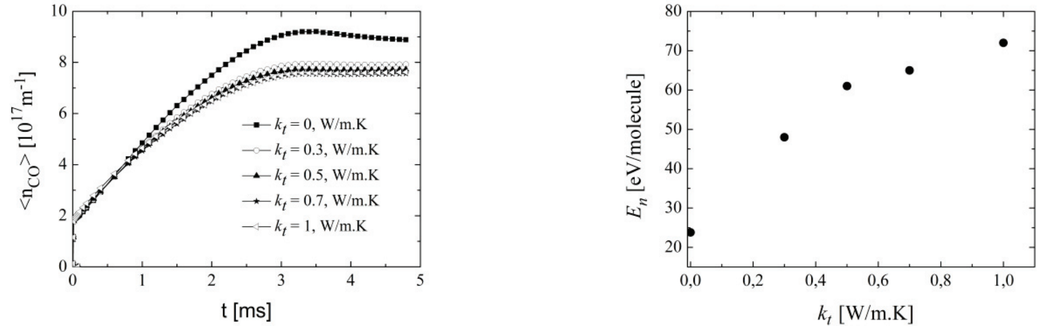


(a)

(b)

FIGURE 3. Radial distribution of the n_e (lines) and the T_g (symbols) at position Y = 10 mm (the arc center) at t = 1 ms in (a) and the energy efficiency of the dissociation of CO_2 in (b) at different values of the parameter k_t.

The total number of CO molecules per unit length of the arc, i.e. the integrated values of the CO density $<n_{CO}>$ over the cross section at different moment of time are shown on Fig. 4(a). They grow in time by forming a plateau after the arc extinguishing time. This is actually the amount of produced CO. The presence of turbulence decreases $<n_{CO}>$ about 1.3 times. The main reason for the reduction of the energy efficiency is the growth of the actual energy cost of one CO molecule produced in a plasma system. The E_n in our simulation (Fig. 4(b)) increases from 24 to 72 [eV/molecule].



(a) (b)

FIGURE 4. The spatially integrated values of the density of CO at different moments of time in (a) and the actual energy cost of one CO molecule produced in the plasma system at different values of parameter k_t in (b).

CONCLUSIONS

Simulations of the influence of the turbulent thermal conductivity on energy efficiency of the CO_2 conversion in GAD have been performed. The results show that at discharge current about 20 mA, the introduction of the turbulent thermal conductivity of 1 W/m.K is not sufficient to cool the gas to an optimal temperature for efficient CO_2 dissociation. The influence of additional factors that could affect gas cooling, such as the relative velocity of the gas flow with respect to the arc, will be investigated after expanding the model.

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REFERENCES

1. A. Fridman, *Plasma Chemistry* (Cambridge University Press, Cambridge, 2008), pp. 200-208.
2. T. Nunnally, K. Gutsol, A. Rabinovich, A. Fridman, A. Gutsol and A. Kemoun, J. Phys. D: Appl. Phys. **44**, 274009 (2011).
3. A. Indarto, D. R. Yang, J. W. Choi, H. Lee, H. K. Song and J. Hazard. Mater **146**, 309-315 (2007).
4. S. R. Sun, H. X. Wang, D. H. Mei, H. Tu and A. Bogaerts, Journal of CO_2 Utilization **17**, 220-234 (2017).
5. W. Wang, D. Mei, X. Tu and A. Bogaerts, Chem. Engineering Journal **330**, pp. 11-25 (2017).
6. W. Wang, A. Berthelot, St. Kolev, X. Tu and A. Bogaerts, Plasma Sources Sci. Technol. **25**, 065012 (2016).
7. G. Trenchev, St. Kolev, W. Wang, M. Ramakers and A. Bogaerts, J. Phys. Chem. C 121, 24470-24479 (2017).
8. St. Kolev, S. Sun, G. Trenchev, W. Wang, H. Wang and A. Bogaerts, Plasma Processes and Polymers **14**, 1600110 (2017).
9. F. R. Menter, M. Kuntz and R. Langtry, Turbulence Heat and Mass Transfer **4**, (2003).