Computer Simulation of PFC Abatement: Mechanisms and Neutral Transport

Thrust A Teleconference

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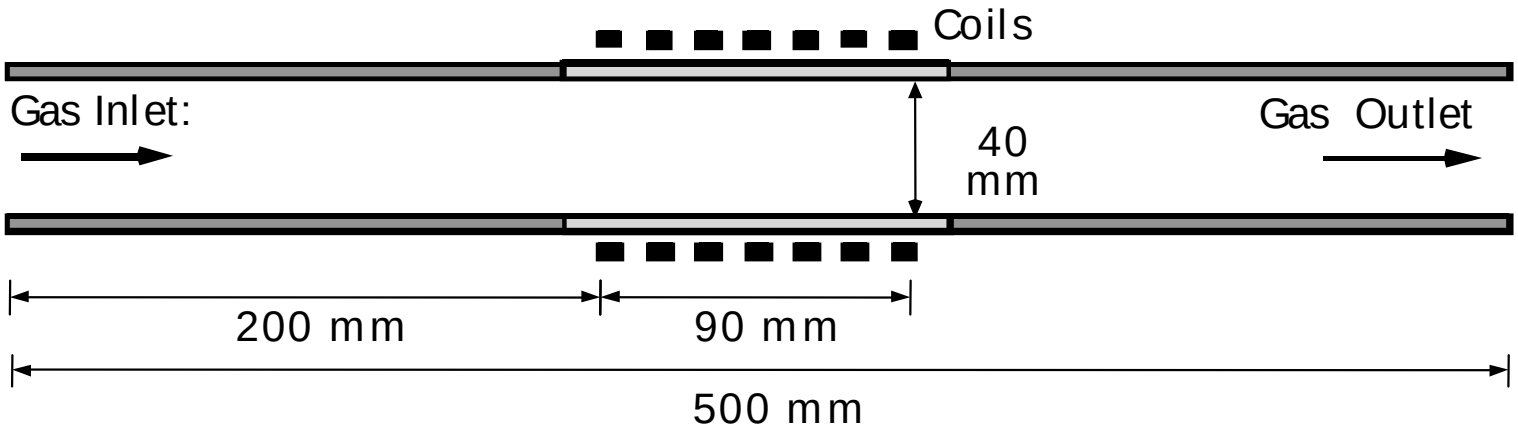
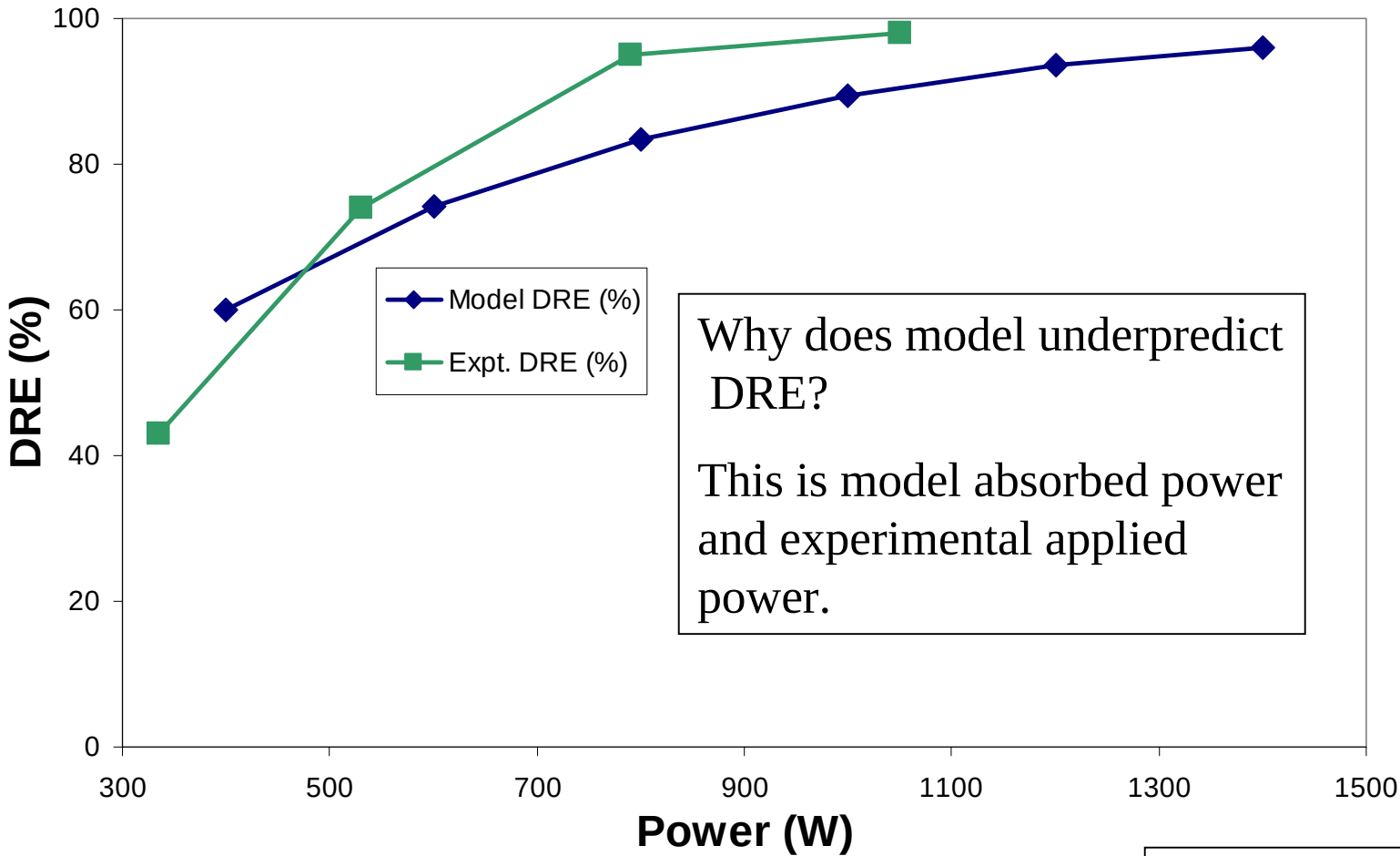
Model Geometry and Formulation



- IC power = 200-1400 W; outlet pressure = 50,100,200,500 mtorr; 2 different coil geometries. Input gas flow = 50/100 sccm CF_4/O_2.
- 2-D (r,z) fluid plasma/neutral model with azimuthal symmetry.
- Electron/ion continuity; ion momentum; electron energy, T_i=0.2 eV.
- Helmholtz, Poisson equations.
- Neutral overall mass, momentum and energy balances.
- Stefan-Maxwell multicomponent diffusion relations solved for N_s species.
- N_s-1 species mass balances.
- Coupled to plasma model via species (chemistry), momentum and energy collisional source terms.
- 8 charged & 14 neutral species. 65 gas phase & 3 surface rxns.

Destruction Efficiency vs. Power for CF_4/O_2 Abatement

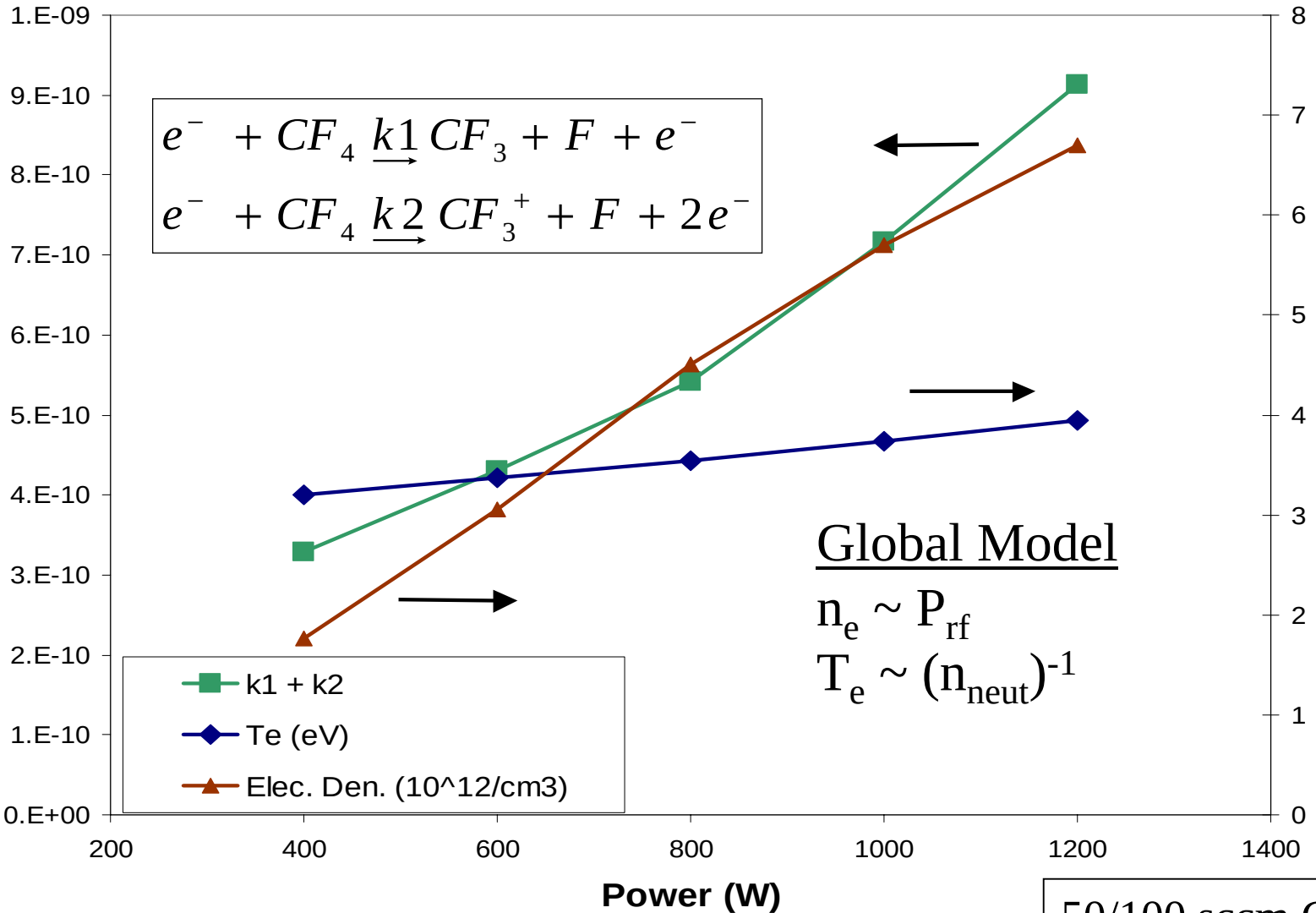


Why does model underpredict DRE?

This is model absorbed power and experimental applied power.

50/100 sccm CF_4/O_2
Pressure = 100 mtorr

The Effect of Power on CF4 Dissociation



50/100 sccm CF_4/O_2

Abatement Mechanisms

- Abatement is governed by CF_4 destruction. Only 6% of dissociated CF_4 ever recombines (CF_x is "burned" by O).

  How do we maximize CF_4 dissociation?

- $R_{CF4} = k*N_{CF4}*Ne$
  - $k=f(T_e)$, so maximize T_e by minimizing N_{neut} through high T_n and low pressure.
  - Maximize N_{CF4} in plasma zone. High T_n promotes diffusion, however diffusive flux to plasma zone of CF4 ~ 1-10% of convective flux.
  - Maximize N_e by high plasma power.
- Plasma expansion with power counters increased neutral velocity (residence time ~ constant).
- Ion neutralization at walls dominates gas phase neutralization for CF_x^+ ($R_{surface} \sim 5*R_{gas}$).

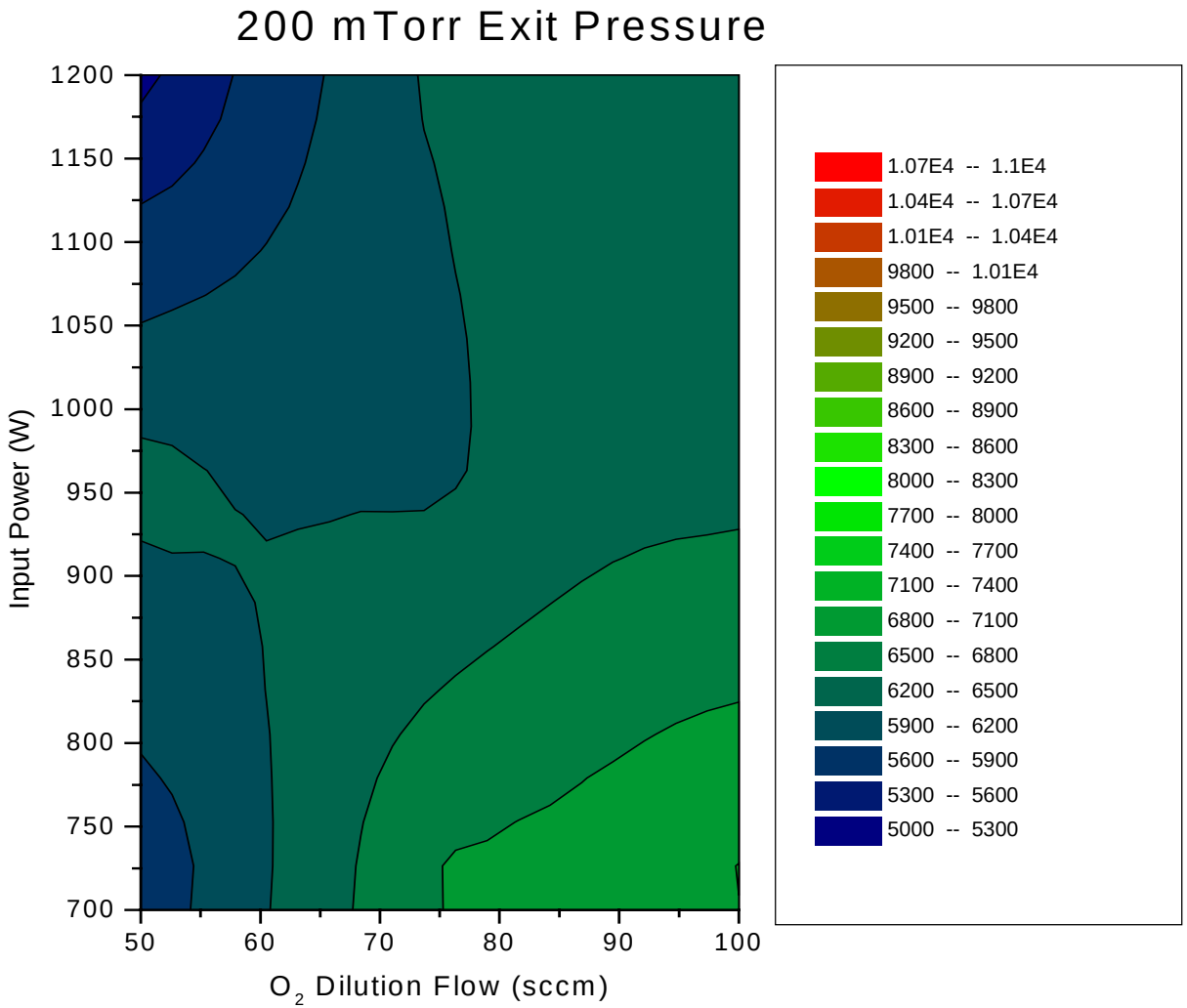
Effect of Input Parameters

Power: Increases N_e, T_n, T_e. N_e spreads axially to maintain residence time in plasma zone. Abatement increases.

Pressure: Decreases T_e, slightly increases N_e and T_n. Abatement decreases.

Coil Spacing: Decreases peak T_e and N_e but lengthens plasma zone. Abatement is unchanged. Shift product distribution towards CO vs. CO_2.

Experimental Results: Abatement Plasmas



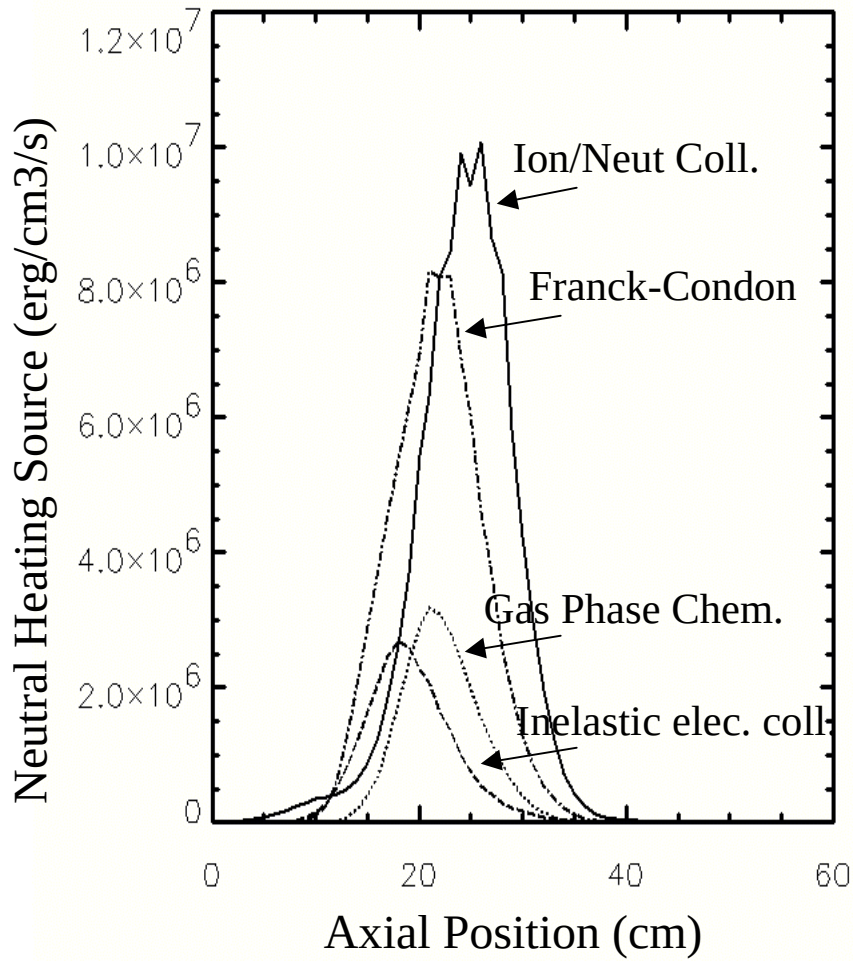
Experimental rotational temperature of C_2 are 5000 - 10000 K.

This is a measurement of the roto-vibrational structure of emission from electronically excited states.

Is this indicative of the true neutral temperature?

Neutral Heating in the Abatement Model

- Ion-Neutral elastic & charge exchange collisions.
- Franck-Condon effects from electron impact dissociation.
- Gas phase thermochemistry.
- Electron impact vibrational excitation of neutrals.
- Surface chemistry.
- How much of ion & electron energy flux to wall returns to plasma?
- What is proper treatment of wall T_n and velocity BCs?



50/100 sccm CF_4/O_2
Power = 1200 W
Pressure = 100 mtorr

Wall Boundary Conditions

- At low densities, continuum conditions no longer apply. We can mitigate the effect of this through "slip," or "jump" BCs at surfaces.
- This also partially decouples the neutral temperature solution from the unknown wall temperature BC.

V Slip	T Slip	DP (mtorr)	Tn (K)	DRE (%)	T Jump (K)	Vel. Jump (cm/s)
No	No	90	1700	80	0	0
No	Yes	112	2083	89.4	405	0
Yes	Yes	95	2062	89.5	402	1811
Experiment		117 ?	?	98.3	?	?

R_{mod}=2 cm R_{expt}=2.54 cm
L_{mod}=59 cm R_{expt}=38 cm

50/100 sccm CF_4/O_2
Power = 1000 W
Pressure = 200 mtorr

Surface Processes and Neutral Temperature

$$\textit{Ion}\ \text{Energy to Walls} = \sum \Gamma_{ion}(\Phi_{sheath} + \Phi_{ionization}) * SA$$

$$\textit{E}\text{lectron Energy to Walls} = 2 * T_e * \Gamma_{electron} * SA$$

$$\textit{Surface}\ \text{Reaction Energy at Walls} = \sum \Delta H_{rxn} * R_{rxn} * SA$$

- Deposit 25% of this energy into neutral source term in finite difference cell nearest wall.

  Original S_{neut} = 260 W

  Ion S_{neut} = 135 W (55% KE, 45% PE)

  Electron S_{neut} = 30 W

  Surface S_{neut} = 25 W

  New S_{neut} = 451 W

Tn increases from 2062 to 2411 K
DP increases from 95 to 113 mtorr
DRE increases from 89.5 to 92%

Bounding Neutral Temperature

- Since the neutral source terms are non-quantitative, but the temperature for a given source amount should be reasonable, we can bound T_n by arbitrarily multiplying the source term by a factor at all points in the model.

Source Term Multiplier	Tn (K)	DRE (%)	DP (mtorr)	S_{neut} (W)
1	2062	89.5	95	260
2	3055	92.9	138	530
2.5	3522	93.7	157	660.2
3	4009	94.4	175	793
1, with 25% of wall energy	2411	92	113	451

Generality of Abatement Results

- HDP tools generally treated as nearly isothermal at Tn ~ 300 - 600 K.
- Abatement plasmas are quite different than, e.g. industrial HDP etch tools.
  - Aspect ratio and large radial and axial gradients
  - Higher pressure
  - **Higher plasma densities**
- At more typical plasma densities, N_e~7*10^{11}, do we see the same effects?

  DRE = 42%, T_n = 1408 K, DP=48 mtorr

  V_{max}/V_{in} = 3.8

Conclusions

- PFC abatement is governed by initial electron impact destruction of PFCs (high power, high T_e, T_n).
- PFC abatement plasmas have large gradients in temperature, velocity and density. How large is large?

Future Work

• Simpler plasmas on experimental system with better diagnostics. Comparison to experiment for N_e, T_e, radical densities etc. should allow iteration towards a "state of the art" model of: O_2, CF_4, CF_4/O_2 plasmas with better treatment of surface and gas phase chemistry and mechanisms of plasma/neutral energy transfer.

•Better abatement models.

• What is the neutral temperature in a high density plasma? Does it impact performance?

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