

The background of the slide is a panoramic view of Xi'an, China, showing a mix of traditional architecture and modern high-rise buildings. The Great Wall of China is visible in the distance.

# 西安 IDCOMP 2019

2019年第一届电力装备绝缘与放电计算学国际研讨会

2019年7月28日~31日

350 participants  
7 pays  
173 présentations

4 participants hors Asie : Zhuoxiang Ren (Geeps), J. Yan and M.Fang (UK), Y. Cressault (Laplace)

2 ½ journées  
20 plenary talks  
4 sessions parallèles/jour (12' par talk)  
95% des présentations en chinois

9 topics : academic and industrial presentations

Arcs-Sparks discharges  
Corona discharges  
Pressure discharges  
Multiphysics computation  
Insulation materials  
SF<sub>6</sub> replacement  
Streamers and breakdown  
Discharges interactions with insulated materials  
Discharge surface and diagnostics  
+ 2 workshops COMSOL+SIMDROID

Point de vue personnel sur l'évolution de la recherche sur les appareillages de coupure et leur simulation

De 1985 à 1995 : modèle hybride, méthodes intégrales et différentielles

### 1<sup>er</sup> constat : les données

Incertitudes sur les propriétés des gaz : transport et NEC (larges différences parfois au niveau des calculs théoriques, encore plus lorsque l'on compare le NEC aux mesures expérimentales)

### 2<sup>ème</sup> constat : les modèles

Modèle d'arc basé sur hypothèse non-LTE avec « laminar flow » ne permet pas d'estimer correctement la RRRV

Plusieurs exemples sont donnés sur les lois de mélanges, NECs et transport avec les différences, avec différents codes de simulation utilisés pour simuler les appareils : k-epsilon, chem-kim, RNG, realisable k-epsilon model, mixing length turbulence model (son préféré)

### Futur :

Vérifier expérimentalement les propriétés radiatives et les propriétés de transport

Estimer l'ablation de PTFE sous l'effet du rayonnement

Confirmer ou infirmer que  $\rho * C_p$  est suffisant pour déterminer de l'efficacité de coupure d'un gaz

Les méthodes conventionnelles ne sont pas valables à haute  $T^\circ$  (>20kK) et hautes pressions (surtout la conductivité électrique)

Modèles 2T non adaptés actuellement si non prise ne compte du champ électrique dans la détermination de la EEDF

Depuis quelques années, augmentation de la puissance et vitesse de calcul des ordinateurs

Coût d'une simulation en Chine : 0.1RMB par CPU heure (0.7€/h)

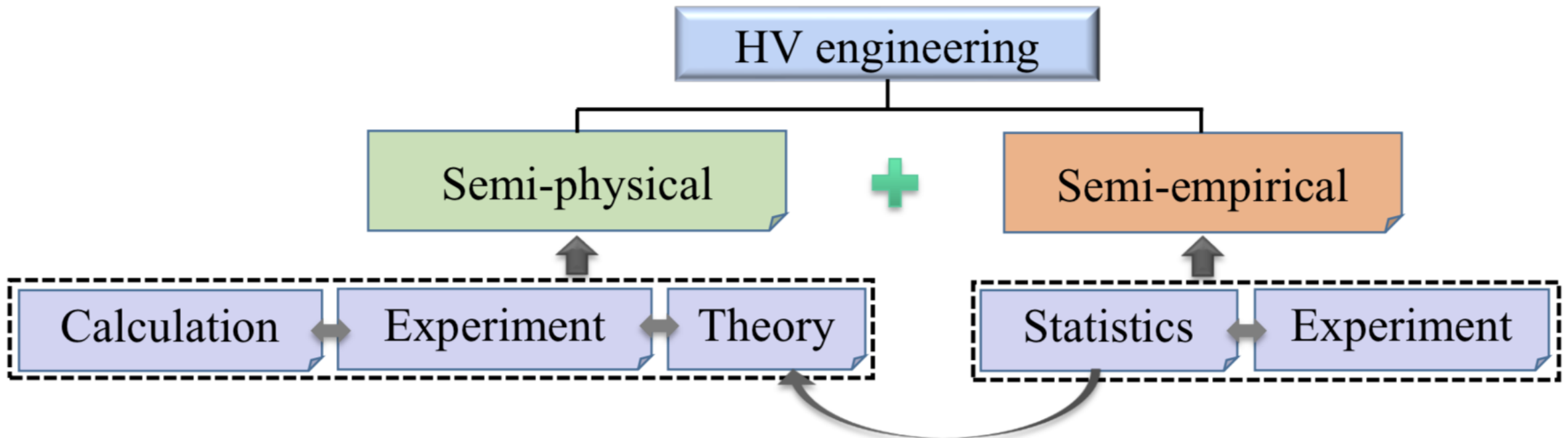
Utilisation prononcée de la CHVE dans le domaine de la biologie et de la mécanique, pourquoi pas dans le HV

### **CHVE = HV + Computer science + Applied physics**

Adaptable aux interfaces gaz/liquides/solides/décharges

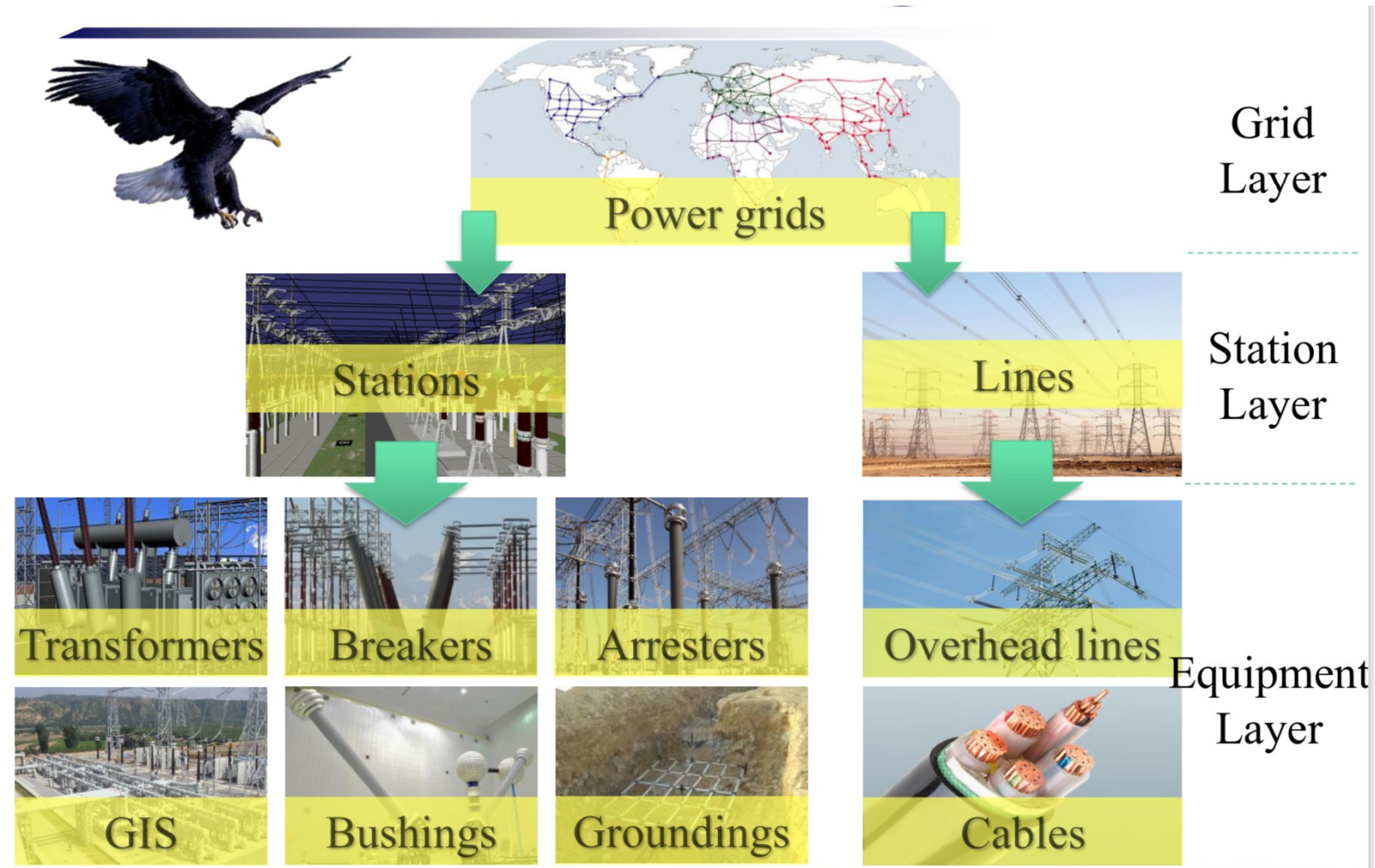
Adaptable à la fabrication et caractérisation des matériaux d'isolation

Adaptable au couplage de phénomènes multiphysiques

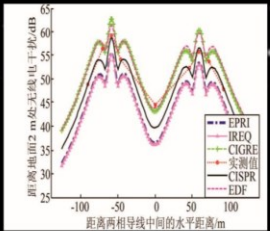


### Objectif de l'entreprise :

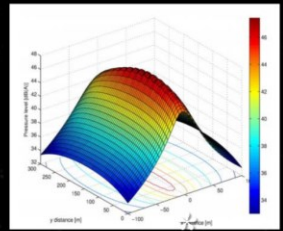
Créer un grid layer (solar, storm, ice, external phenomena) + station layer (electromagnetic field) + equipment layer ( )



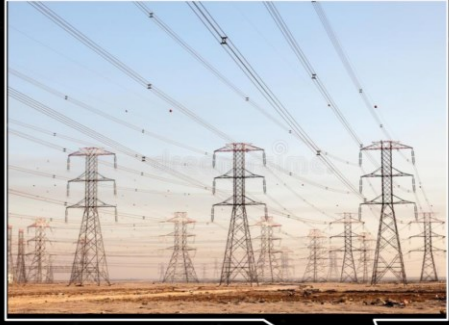
### EM interference\*



### Noise distribution\*\*



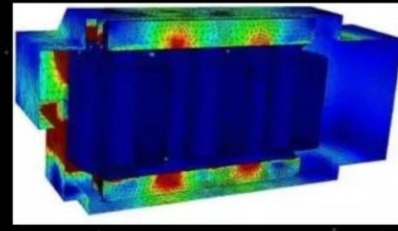
### Transmission Lines



### Lightning strikes on lines



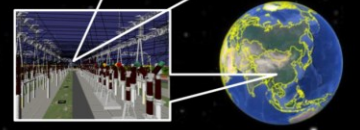
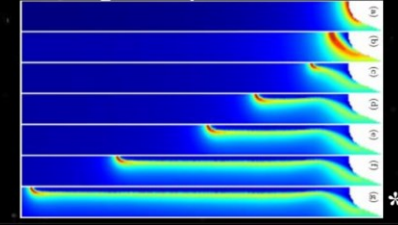
### Electromagnetic, fluid, thermal, mechanic field



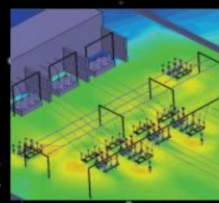
### Transformers



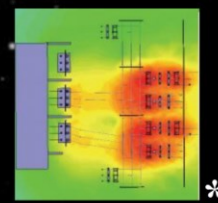
### Discharge in liquid and solid material



### Electric field



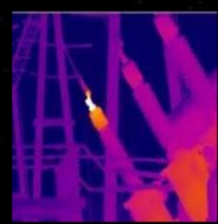
### Magnetic field



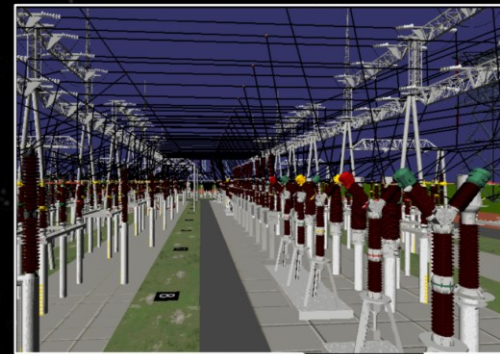
### Lightning stroke



### Thermal field



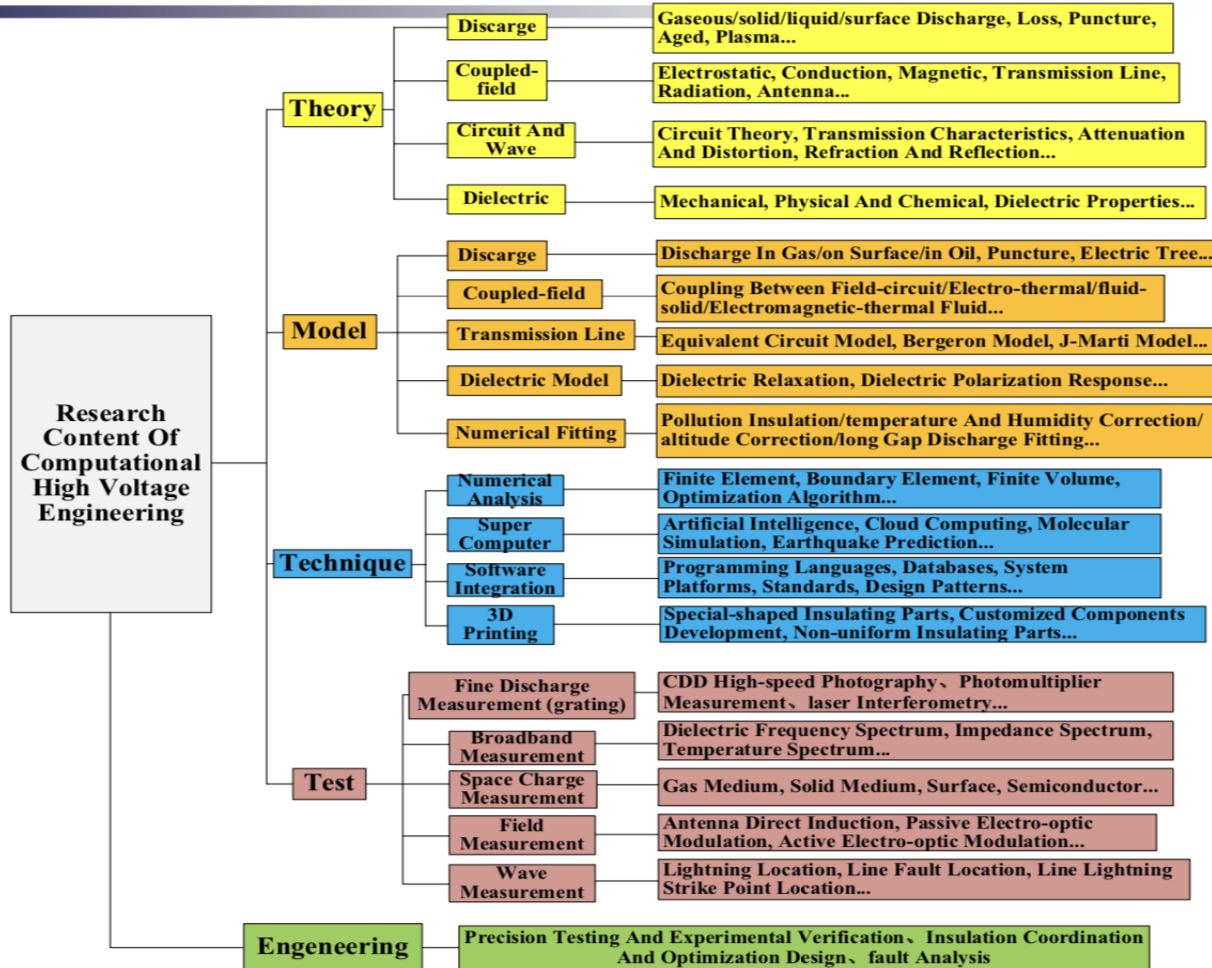
### Substation/Converter station



### Earthquake



### 3. CHVE Architecture



### 3. Architecture of CHVE – Testing

- ◆ To measure **electrical, thermal, mechanical** and **micro parameters** of dielectric materials for the models.

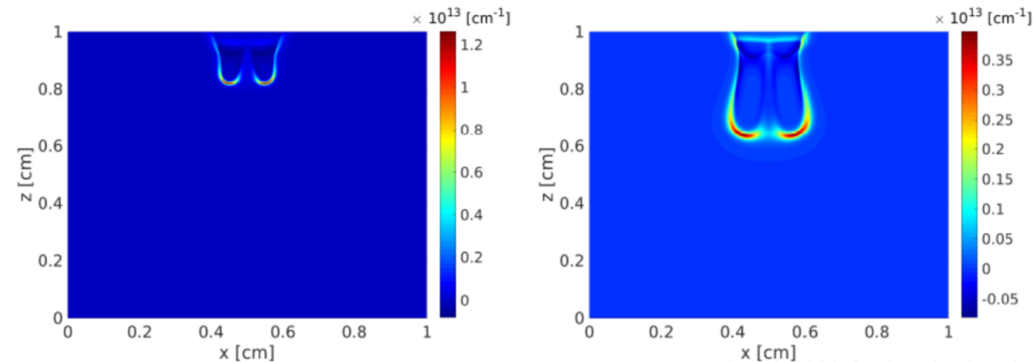
Electrical	Thermal	Mechanical	Micro
Rated parameters, Electrical conductivity, Magnetic permeability, Dielectric constant, Charge density, B-H curve, Electric field, Magnetic field	Specific heat capacity, Thermal conductivity, Emissivity, Dynamic viscosity, Kinematic viscosity, Boiling point, Melting point, Coefficient of thermal expansion, Temperature	Modulus of elasticity, Poisson's ratio, Shear modulus, Yield strength, Tensile strength, Ductility, Toughness, Hardness, Fatigue strength	Electron mobility, Free path, Electron lifetime, Fermi level, Recombination rate, Bond energy parameter, Bond angle parameter

Test sur streamer double-headed – 1s de temps de calcul avec 1000CPU

#### 4.1 3D simulation of streamer discharge \*

(Chijie Zhuang, Tsinghua University)

- ◆ A double-headed streamer was simulated within a cubicle of  $1 \text{ cm}^3$ , with mesh size  $2048 \times 2048 \times 2560$ , which generated 1 billion degrees of freedom in simulation.
- ◆ Tianhe 2-JK in Beijing was used for 3D simulation. The computing time is about 1s when using 1000 GPUs.



#### Challenges pour demain :

- Etude précise de la génération et du mouvement de particules chargées
- Convergence améliorée pour le couplage de différents champs
- Amélioration de la qualité de production



$C_4F_7N$  représente un bon candidat pour remplacer le  $SF_6$  (à cause du N – donc ajout de O ou  $O_2$ )

**Objectif :** Modéliser la production de produits décomposés/formés

**Technique :** Décomposition par la méthode DFT (Density Functional Theory)

Couplage hybride de 2 méthodes : B3LYP Becke, 3-parameter, Lee–Yang–Parr (non-local-density approximation) + TZP (triple-zeta exponential)

### Exemples de chemins possibles

$C_4F_7NO \rightarrow C_3F_4NO + CF_3$  (moyenne énergie nécessaire)

->  $C_3F_5N + CF_2O$  (faible énergie)

->  $C_3F_7O + CN$  (moyenne énergie)

->  $C_3F_3NO + CF_4$  (faible énergie)

->  $C_4F_7O + N$  (haute énergie, difficile)

Faible énergie : 2kcal/mol

Moyenne énergie : 110kcal/mol

Haute énergie : 320kcal/mol

Analyse de deux réactions de décomposition, notées A et D

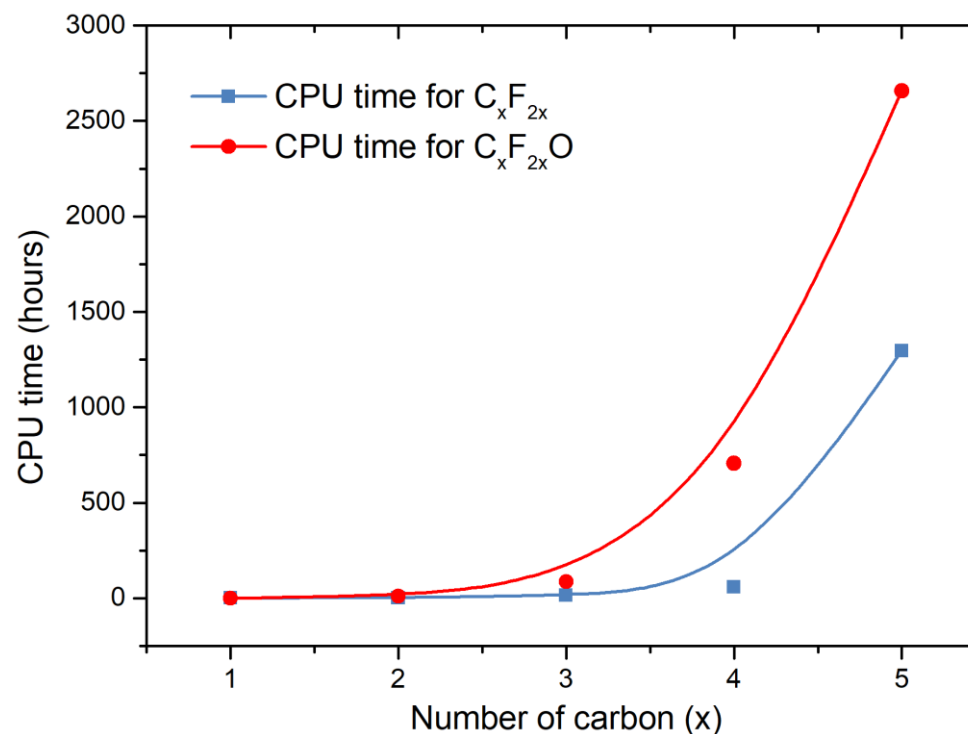
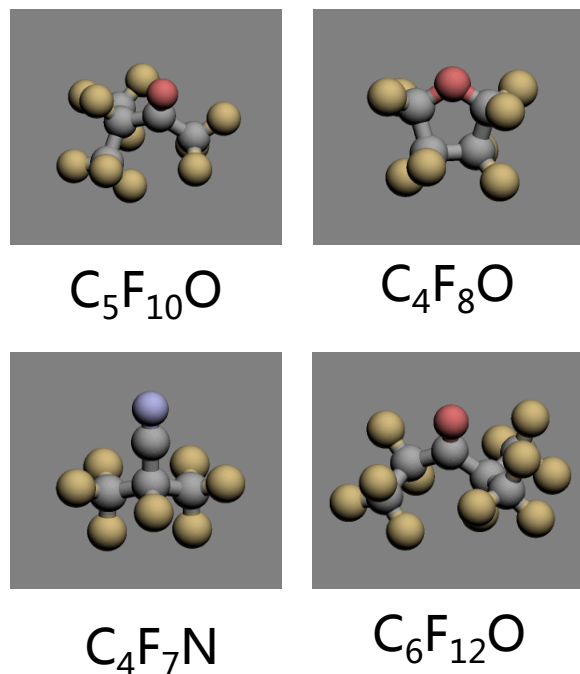
Taux de réactions pour A et B calculés de 300K à 3500K par la méthode TST (transition state theory)

**Part du constat que :**

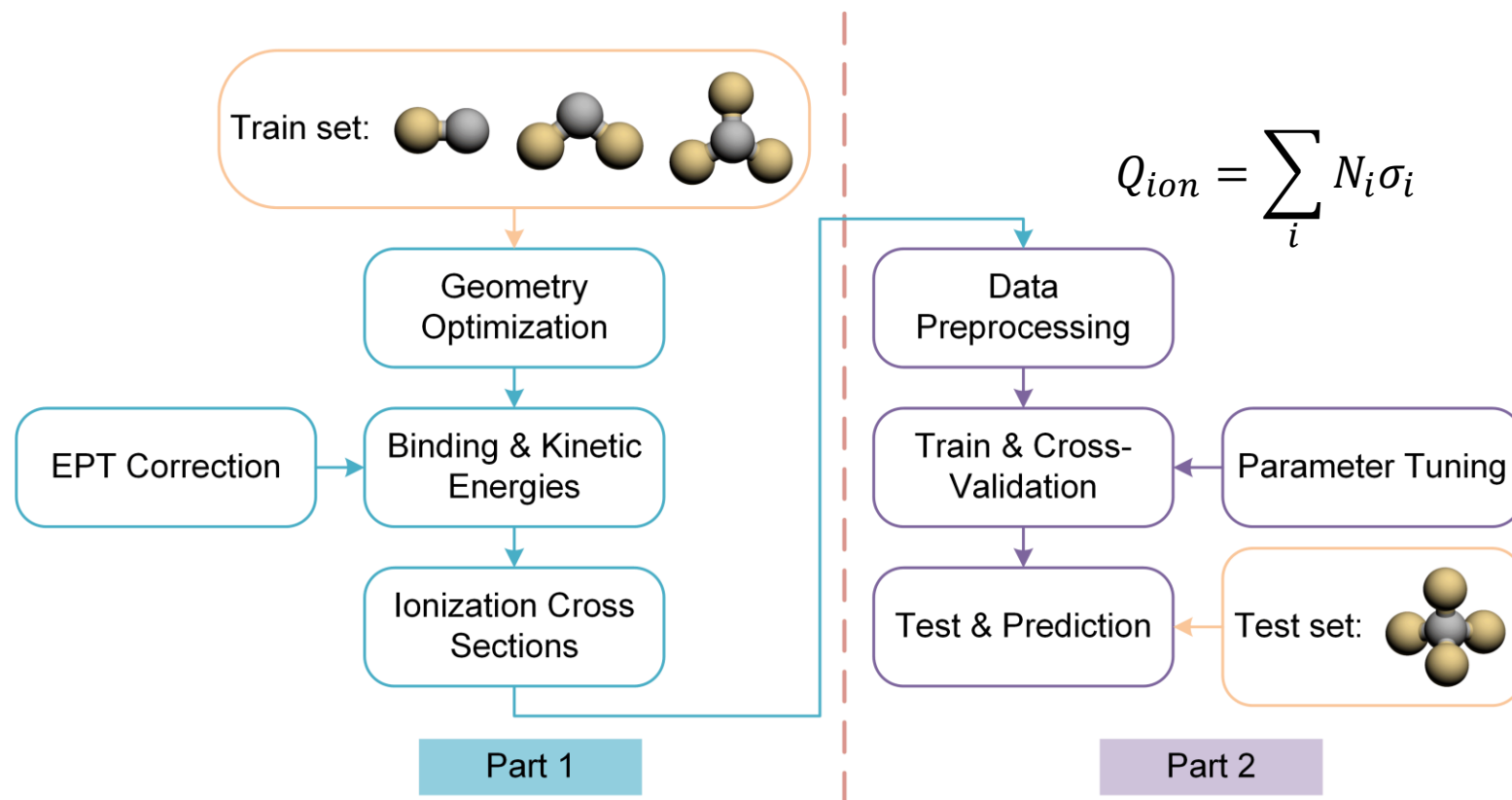
1/ Les collision électrons-molécules (elastic-inelastic excitation, ionisation, attachment) -> processus fondamental pour l'ionisation du milieu

2/ Les sections s'obtiennent par des études expérimentales (chères), ou des calculs théoriques (gourmands en temps de calcul par les méthodes de Binary Encounter Bethe BEB model ou Deutsch-Mark DM model)

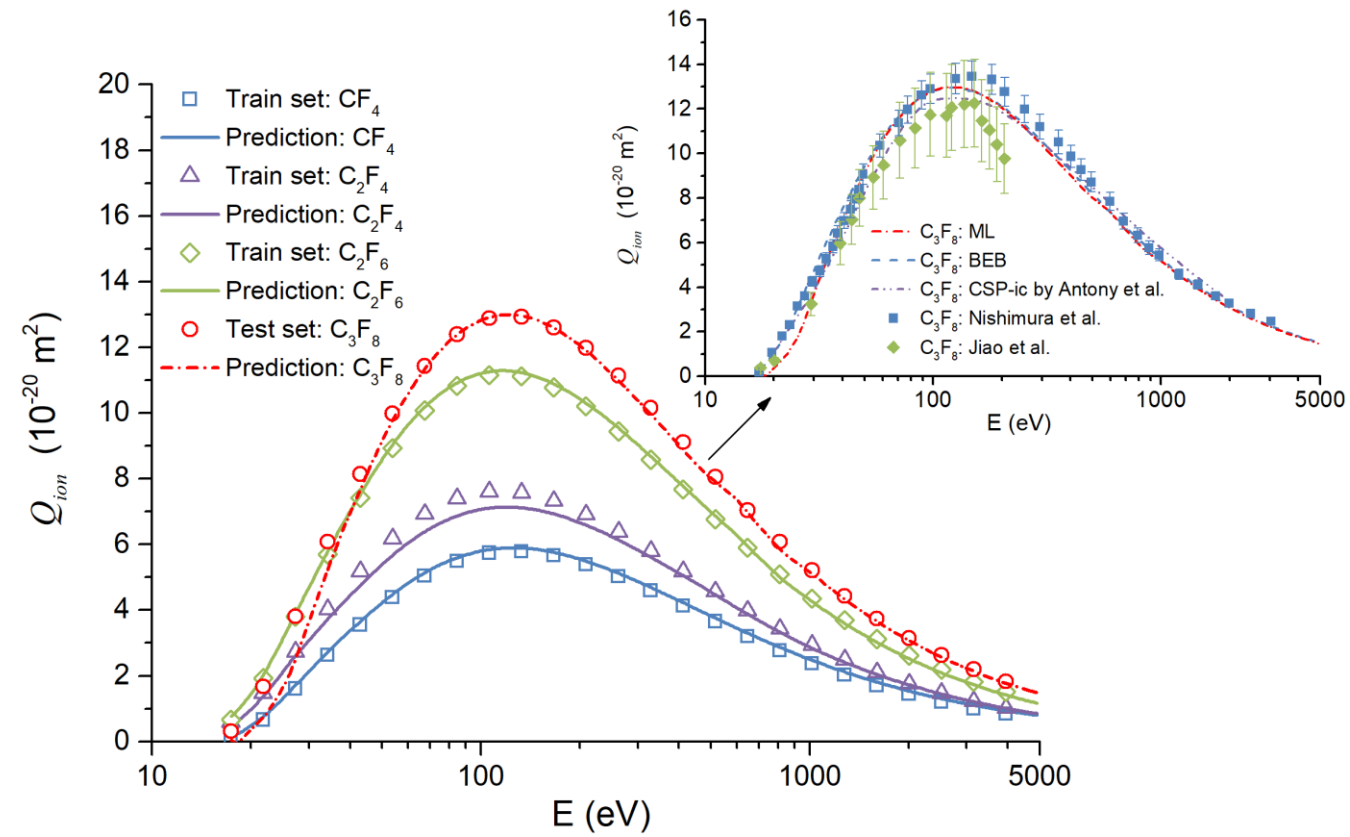
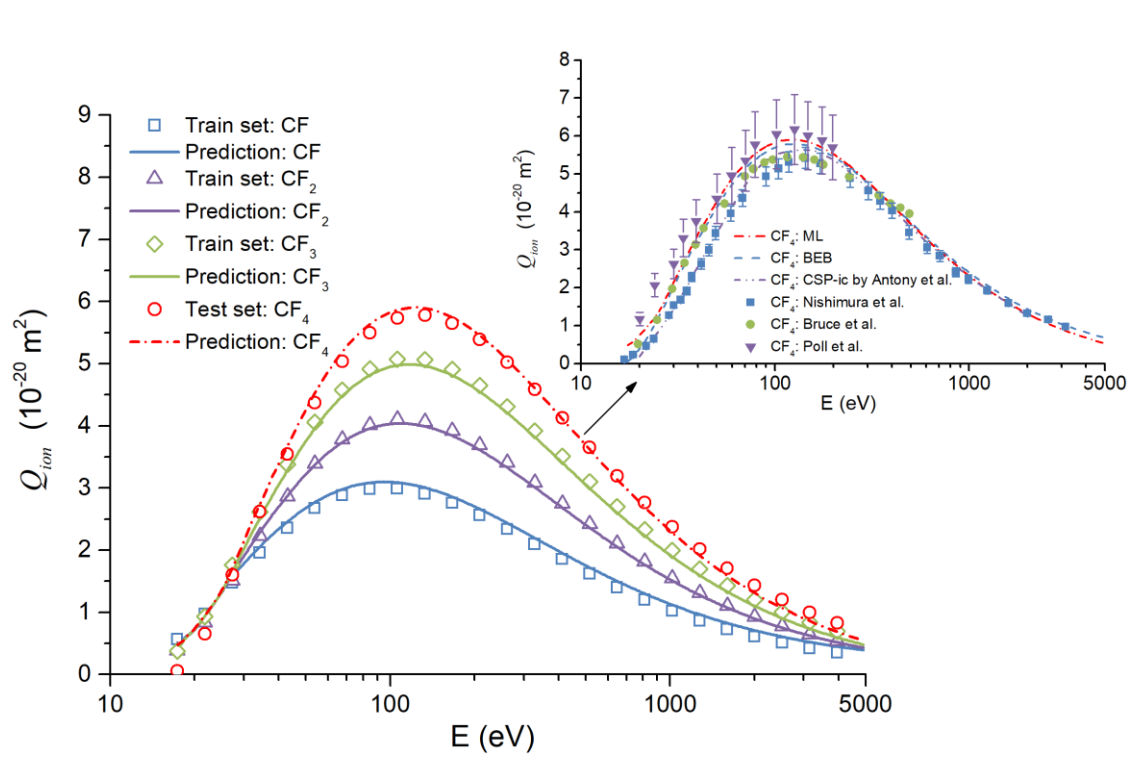
3/ Le temps de calcul augmentent exponentiellement avec le nombre d'atomes de carbones dans la chaîne



4/ Il semble possible de déterminer la section efficace de collision d'ionisation  $Q_{ion}$  de grosses molécules connaissant celle des plus petites qui la composent

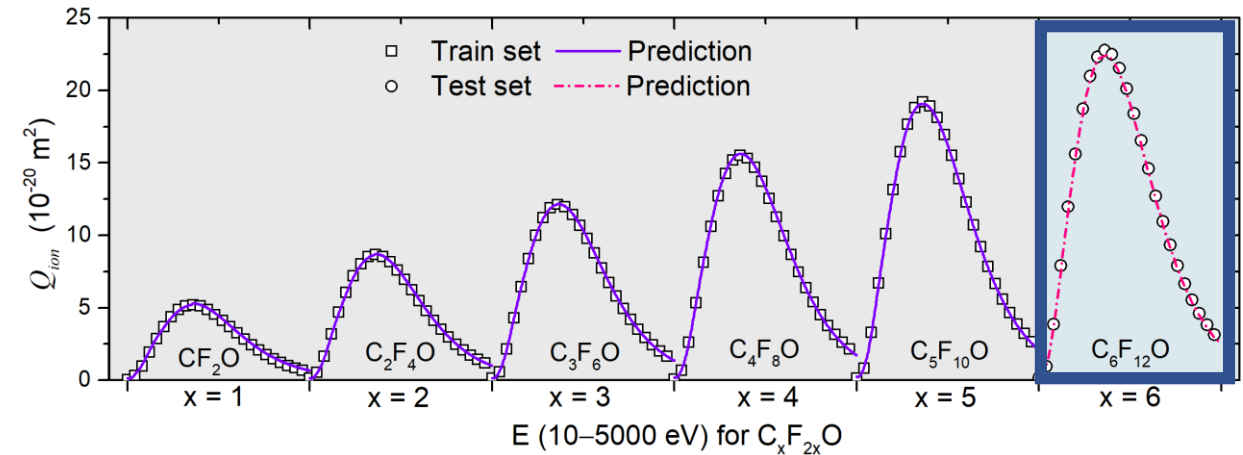
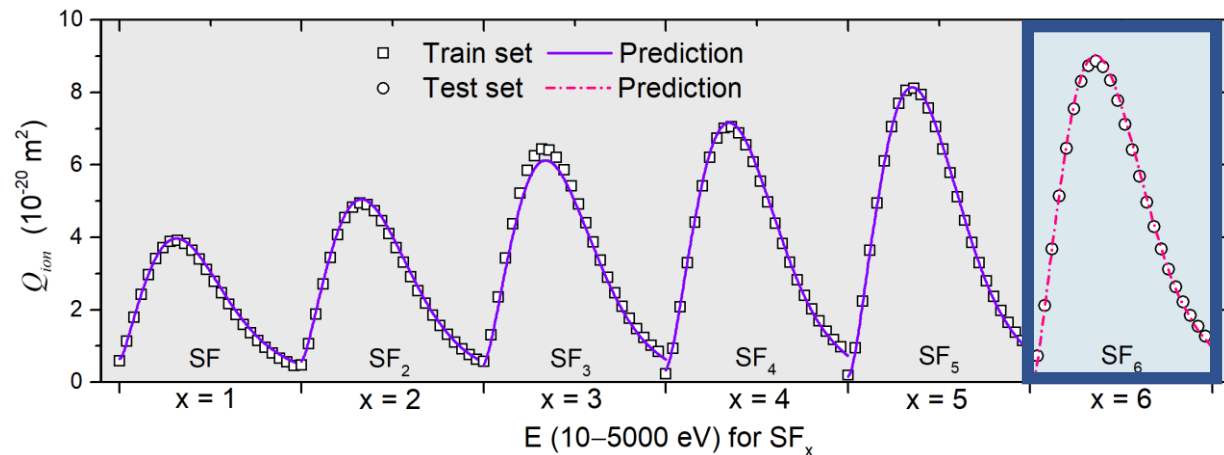
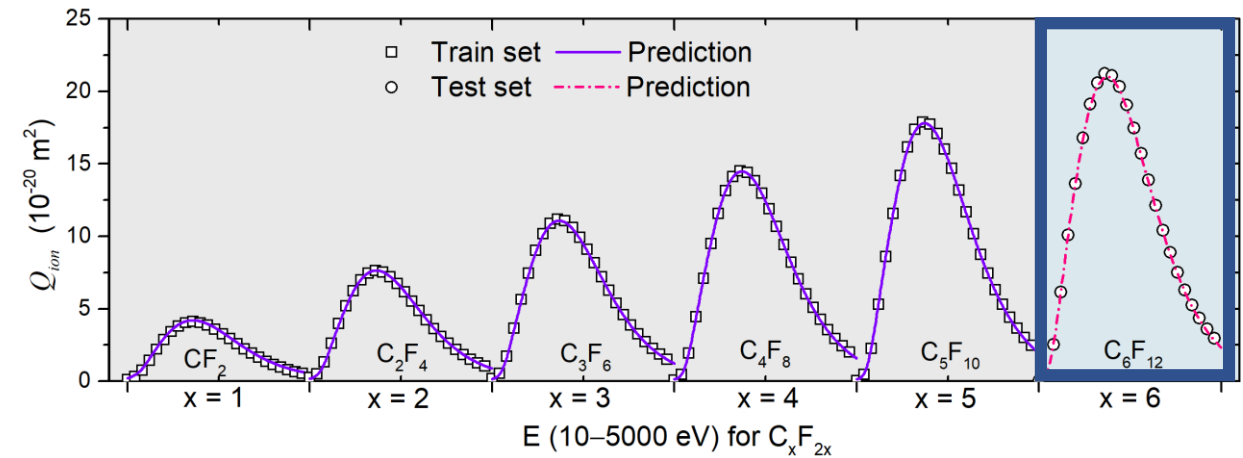
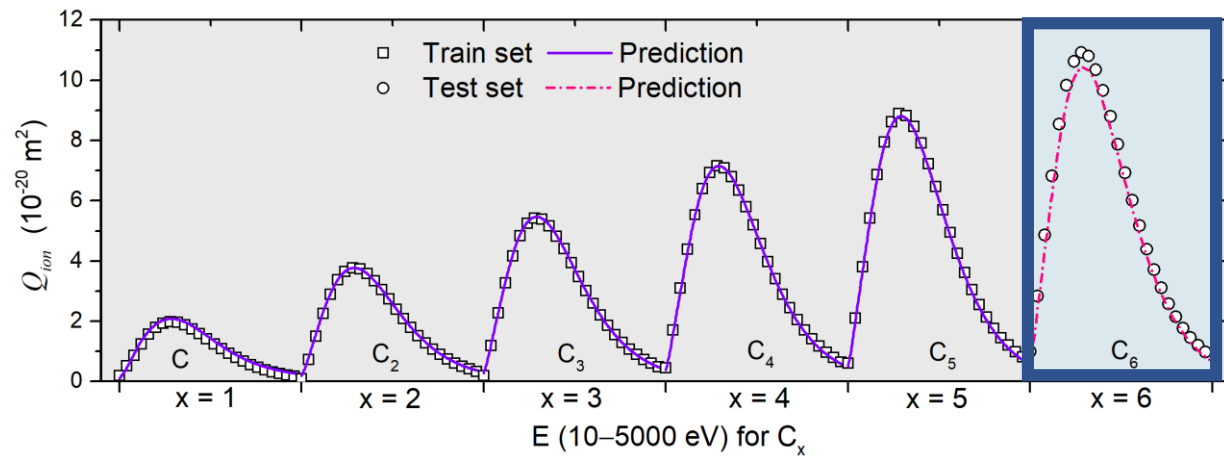


Cette méthode ne donne pas d'expression algébrique pour calculer  $Q_{ion}$  mais apprend du comportement similaires des sections efficaces  $Q_{ion}$  d'autres molécules, en étudiant le comportement de la fonction  $f(\text{incident energy electron})=y_{\text{ionisation cross section}}$



### Part du constat que :

Ca marche, exemples donnés pour 4 molécules complexes :  $C_6$ ,  $SF_6$ ,  $C_6F_{12}$ ,  $C_6F_{12}O$



Dans les applications TIG : les vapeurs métalliques viennent du weld pool - Electrodes en tungsten

### Modèle: TIG dans Helium + vapeurs Fe / Cr

- Les expériences montrent présence de vapeurs proche workpiece mais aussi cathode (déposition de Cr par ex)
- Equations du modèle, utilisation des coefficients de diffusion combinés étendus à des mélanges ternaires (Cr-Fe-He)
- But du modèle : montrer que la diffusion joue un rôle important, coefficient combiné  $D_E$

**Résultats :** Bon accord entre calculs et mesures radialement (basé sur l'émission des raies Cr à 520.8nm)

Sans vapeurs  $T_{max}=21000K$ , avec vapeurs  $T_{max}=13000K$ , la diffusion sous effet du champ électrique est un processus dominant (for upward transport of metal vapor). On observe des vapeurs Cr proche de la cathode, déposées dans des régions où  $T > T_{boil}$

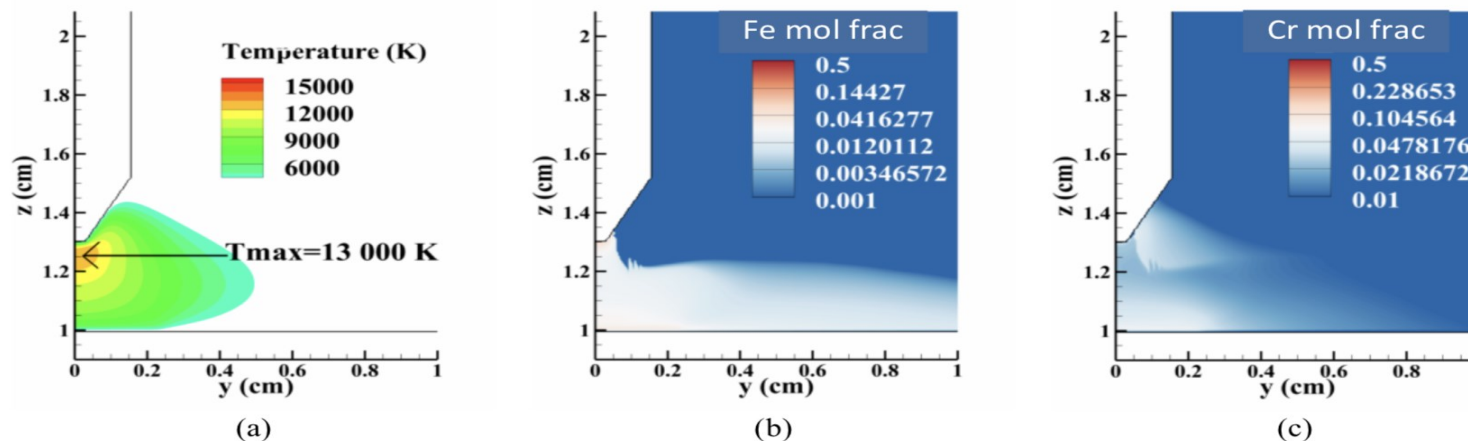


Fig. 4. Distributions of (a) temperature, (b) iron vapour mole fraction and (c) chromium vapour mole fraction in helium TIG welding of stainless steel.

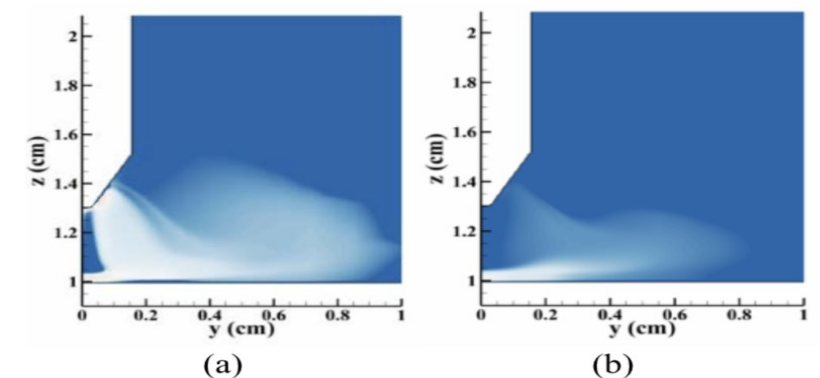


Fig. 2. Distributions of chromium vapour mole fraction neglecting (a) diffusion driven by electric fields and (b) diffusion driven by temperature gradients. The mole fraction scale is the same as in Fig. 1(c).

### Modèle: TIG dans Argon + vapeurs Fe / Cr

- Comparaison faite avec et sans diffusion sous Champ Electric, avec et sans diffusion sous gradient T

### Résultats:

- La diffusion à cause des gradients de températures est dominant (pas par E), plus forte à basses T pour Ar-Fe-Cr que He-Fe-Cr, les coefficients de diffusion combinés  $D_E$  sont plus faibles pour Ar-Fe-Cr que He-Fe-Cr
- Les vapeurs métalliques sont produites à l'anode, puis diffusion **upwards** to recirculating flow, et trapped near cathode tip by upward diffusion -> importance de la convection

Validation par mesures expérimentales : OES montre la présence de Cr proche cathode

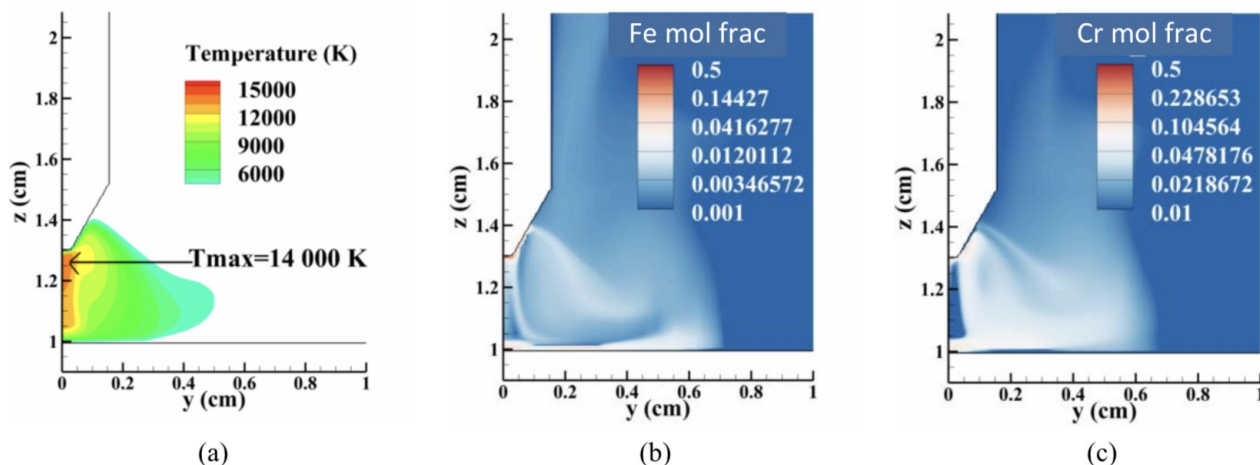


Fig. 1. Distributions of (a) temperature, (b) iron vapour mole fraction, (c) chromium vapour mole fraction in argon TIG welding of stainless steel.

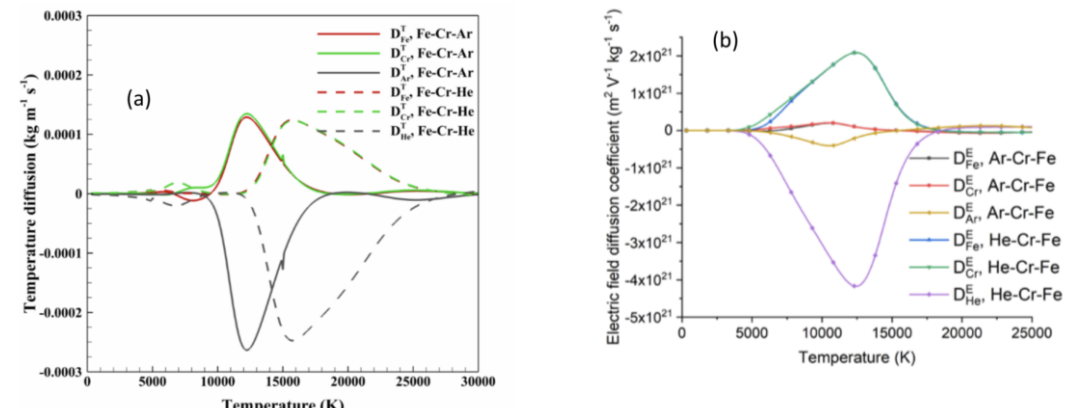


Fig. 3. Combined (a) temperature and (b) electric field diffusion coefficients for mixtures of 10% wt% iron and 10 wt% chromium with argon or helium.



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## Objectifs pour la prochaine conférence

Hors de Chine

Elargir le ISC

Garder les mêmes topics

Mélanges de présentations académiques et industrielles





**SIEMENS**



# Calculation of radiative properties for thermal plasmas : the state of art and outlooks

Y. Cressault, Ph. Teulet, X. Baumann, N. Kabbaj, L. Hermette, F. Reichert, A. Petchanka

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**IDCOMPU 2019**

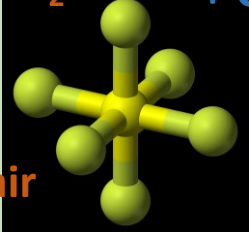
University Toulouse III - Laplace

1953 : High Voltage Circuit Breakers SF<sub>6</sub>

1 Environmental

SF<sub>6</sub>  
CO<sub>2</sub>  
CF<sub>3</sub>I  
C<sub>4</sub>F<sub>7</sub>N  
C<sub>x</sub>F<sub>y</sub>O<sub>z</sub>  
g<sup>3</sup>

+ N<sub>2</sub>  
+ O<sub>2</sub>  
+ air

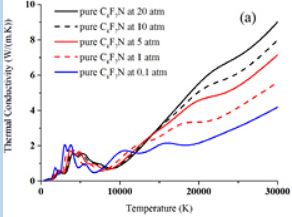
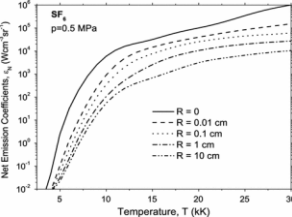


+ CO<sub>2</sub>  
+ Cu  
+ Al  
+ Ag  
Fe

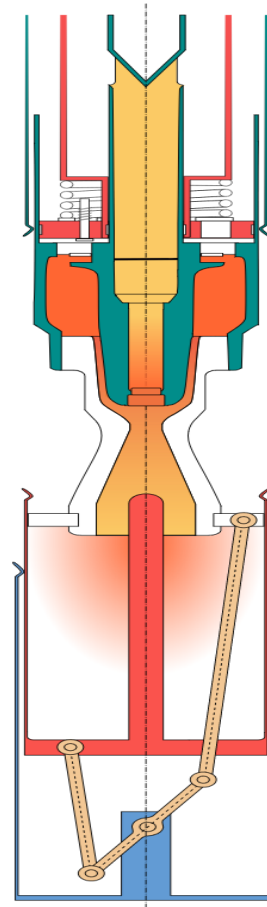
SF<sub>6</sub>, N<sub>2</sub>, Air, CO<sub>2</sub>, SF<sub>6</sub>/N<sub>2</sub>, SF<sub>6</sub>/Air, SF<sub>6</sub>/CO<sub>2</sub>, SF<sub>6</sub>/H<sub>2</sub>, SF<sub>6</sub>/CF<sub>4</sub>, SF<sub>6</sub>/C<sub>2</sub>F<sub>4</sub>, CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>,  
c-C<sub>4</sub>F<sub>8</sub> (+Ar/O<sub>2</sub>/N<sub>2</sub>/CO<sub>2</sub>/CF<sub>4</sub>), CF<sub>3</sub>I (+O<sub>2</sub>/Air/CO<sub>2</sub>), C<sub>4</sub>F<sub>7</sub>N (+N<sub>2</sub>/CO<sub>2</sub>/OH/Cl/O<sub>2</sub>),  
C<sub>5</sub>F<sub>10</sub>O, C<sub>6</sub>F<sub>12</sub>O (+N<sub>2</sub>/Air), CF<sub>3</sub>NSF<sub>2</sub>, CF<sub>3</sub>Cl, CHF<sub>3</sub>, CF<sub>2</sub>Cl<sub>2</sub>, CHF<sub>2</sub>Cl<sub>3-ar</sub>, CHF<sub>2</sub>Cl<sub>3-ar</sub>, C<sub>6</sub>H<sub>2n+2</sub>, CCl<sub>2</sub>F<sub>2</sub> (R12) ...

2 Thermal properties

Composition of the plasmas  
Thermodynamic / transport  
Radiative properties

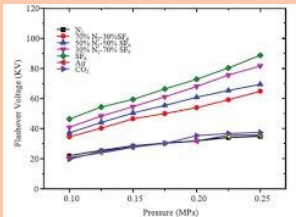
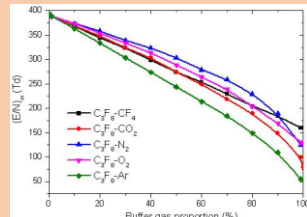
= f(T, P, R, %, LTE or non LTE/LCE)



5 Experiments

3 Dielectric properties

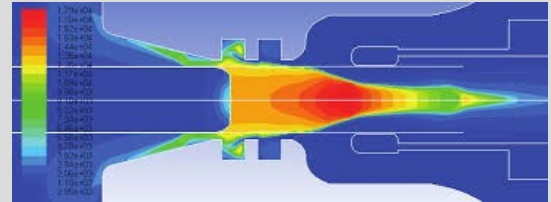
Attachment coefficient  
Ionization coefficient

E/N critical electric field  
Breakdown voltage

4 Numerical model 2D/3D

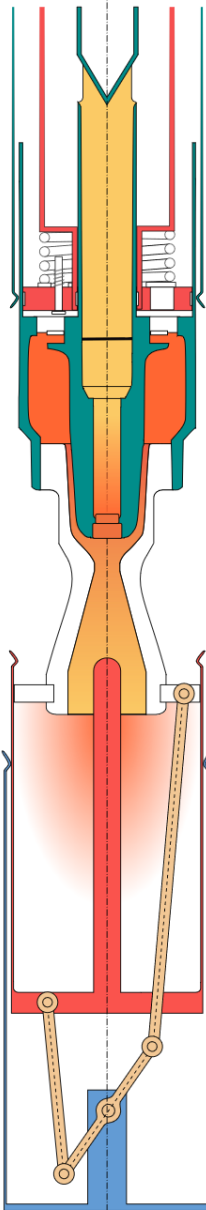
Comsol / Fluent Ansys  
Home code



Ignition, extinction  
Erosion, ablation

## Magneto-Hydro-Dynamic modelling (MHD)

Equations of conservation (mass + transport + energy) + Maxwell equations



$$\frac{\partial(\rho h)}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} h) = \frac{\partial P}{\partial t} + \vec{\nabla} \cdot (\kappa_t \vec{\nabla} T) + \frac{\vec{j} \cdot \vec{j}}{\sigma} + \frac{5 k_B}{2 e} \left( \frac{\vec{j} \cdot \vec{\nabla} h}{c_p} \right) - S_{rad}$$

Mass density  $\rho$  (green arrow), Mass enthalpy  $\rho \vec{u} h$  (red arrow), Thermal conductivity  $\kappa_t$  (green arrow), Electrical conductivity  $\sigma$  (blue arrow), Radiative properties  $S_{rad}$  (yellow arrow pointing to the box).

- ❶ How to treat the radiative losses in hottest regions (strong emission) -> NECs
- ❷ How to treat the radiative losses in intermediate / cold regions (absorption) -> P1 model (MACs) / DOM
- ❸ How to develop the degenerative methods (optimization and comparison with the exact calculation)
- ❹ How to calculate the 2T properties (for the current zero phase for example)

**Radiative losses :**  
Exact solution of RTE

# The Radiative Transfer Equation (RTE)

## Divergence of the Radiative Flux (DRF)

$$S_{rad} = \vec{\nabla} \cdot \vec{F}_r$$

$$\vec{F}_r = \int \int L_\lambda(\vec{r}, d\vec{\Omega}) \cdot \vec{s} \cdot \vec{n} \cdot d\Omega \cdot d\lambda$$

$$\frac{dL_\lambda}{dr}$$

## Radiative Transfer Equation (RTE)

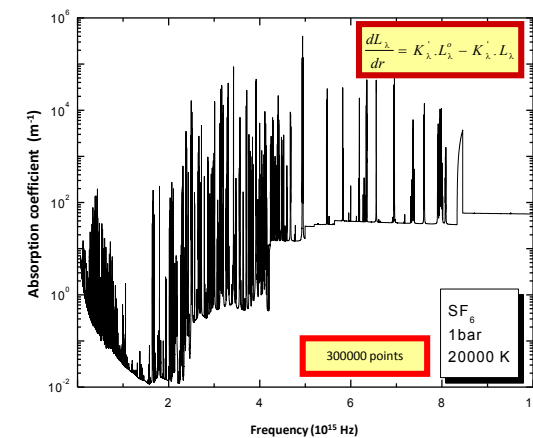
$$\vec{s} \cdot \vec{\nabla} L_\lambda = K_\lambda' \cdot L^0_\lambda - K_\lambda \cdot L_\lambda$$

Directions

T, P, λ

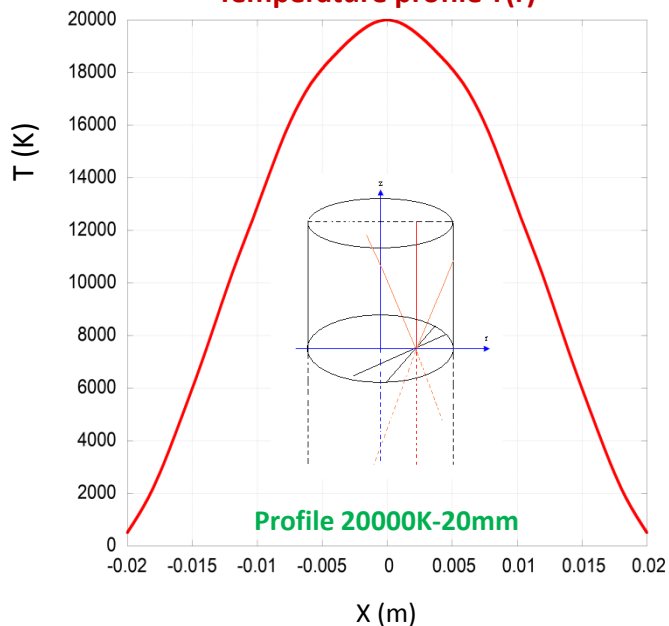
Wavelengths

## Radiative properties

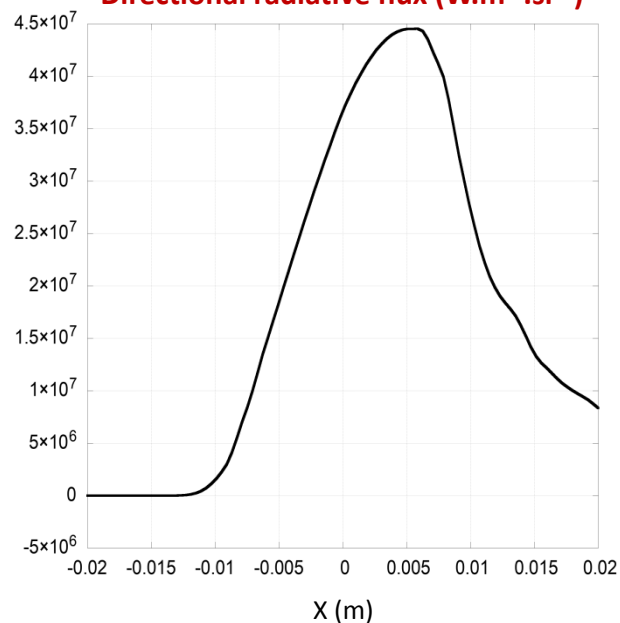


## Resolution of the Radiative Transfer Equation (RTE) – Exact solution

Temperature profile T(r)

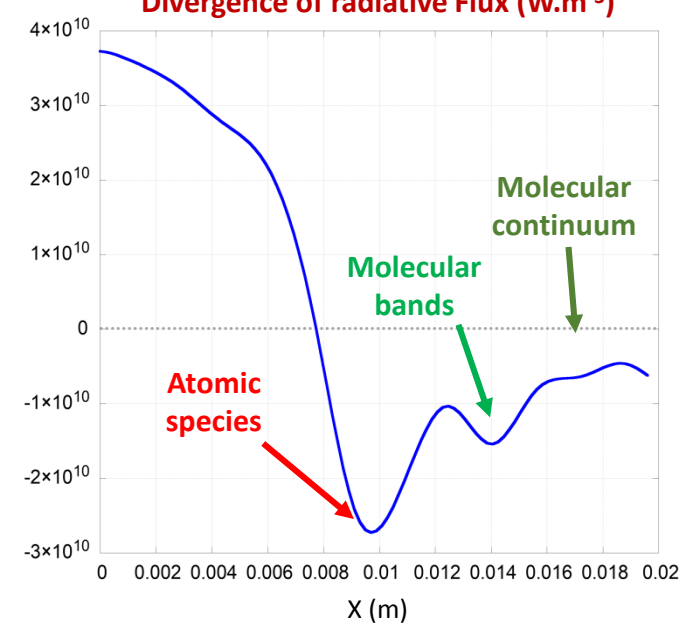


Directional radiative flux (W.m<sup>-2</sup>.sr<sup>-1</sup>)



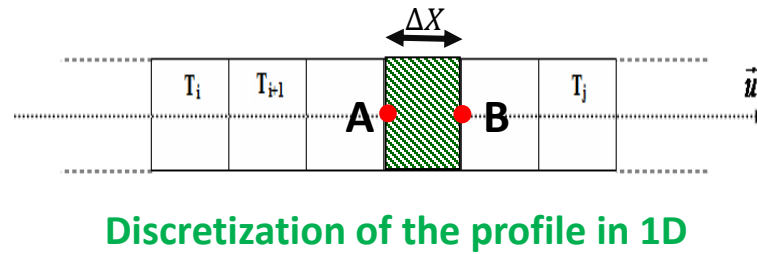
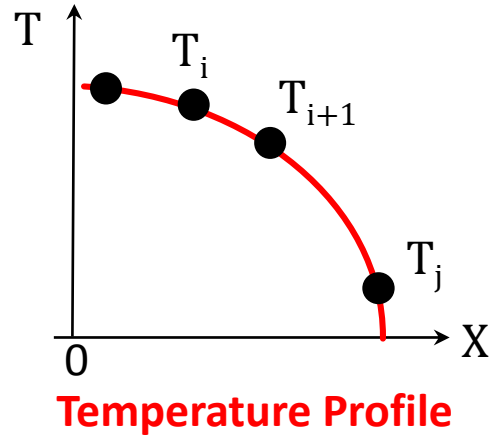
Integration

Divergence of radiative Flux (W.m<sup>-3</sup>)



# The Radiative Transfer Equation (RTE)

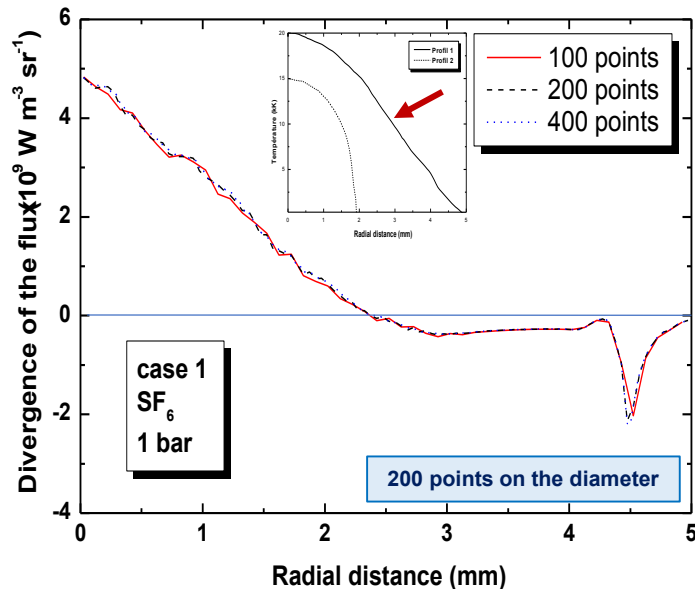
## Solution in 1D of the Radiative Transfer Equation (RTE) – Exact solution



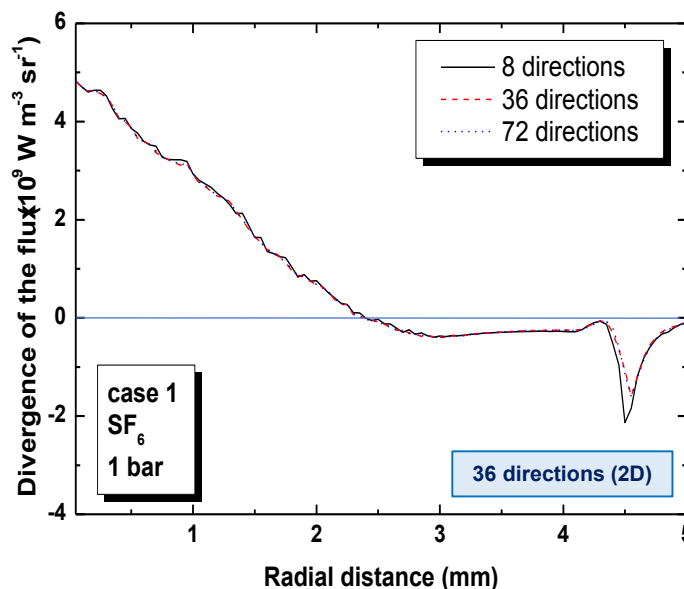
$$L_{\lambda}(i) = L_{\lambda}(i-1) \cdot \exp(-K' \cdot \Delta X) + L_{\lambda}^0(T_i) \cdot (1 - \exp(-K' \cdot \Delta X))$$

Incident at point A (points to  $L_{\lambda}(i-1)$ )  
Directional flux in the point B (points to  $L_{\lambda}(i)$ )  
Absorbed by the cell (points to  $\exp(-K' \cdot \Delta X)$ )  
Emitted by the cell (points to  $L_{\lambda}^0(T_i) \cdot (1 - \exp(-K' \cdot \Delta X))$ )

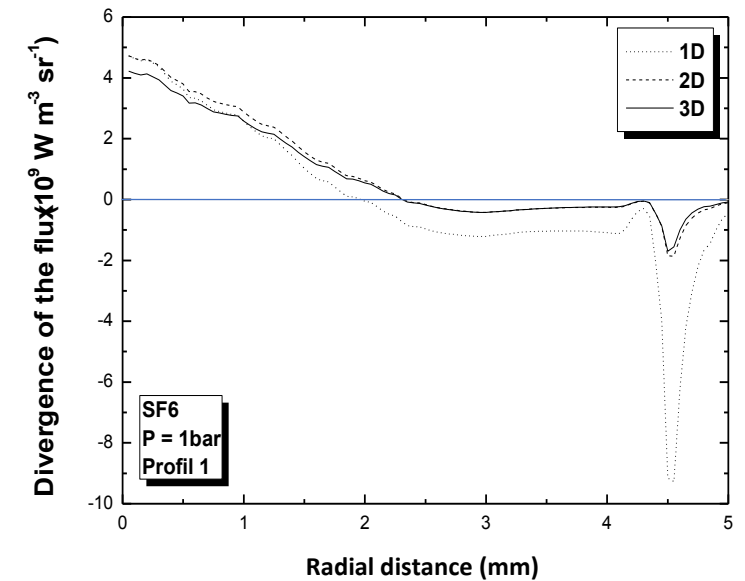
### Influence of the discretization



### Influence of the number of directions



### Influence - 1D/2D/3D



## Radiative losses :

Use of geometrical simplifications  
to solve the RTE

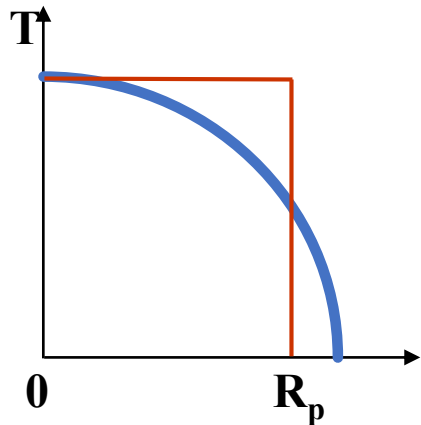
Radiative Transfer Equation (RTE)

$$\vec{s} \cdot \vec{\nabla} L_\lambda = K_\lambda' \cdot L^0_\lambda - K_\lambda' \cdot L_\lambda$$

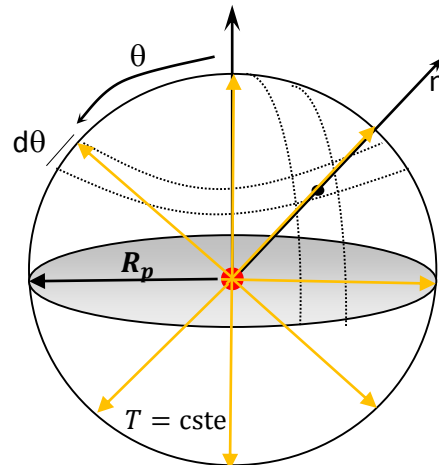


The Net Emission Coefficient (NEC) – Lowke and Capriotti (1969)

Isothermal plasma



Homogeneous plasma



80%-90% of accuracy

Spherical plasma of radius  $R_p$

$$\epsilon_n = \int K'(\lambda, T) \cdot L^0_\lambda \exp(-K'(\lambda, T) \cdot R_p) d\lambda$$

$$\vec{\nabla} \cdot \vec{F} = S_{rad} = 4\pi\epsilon_n$$

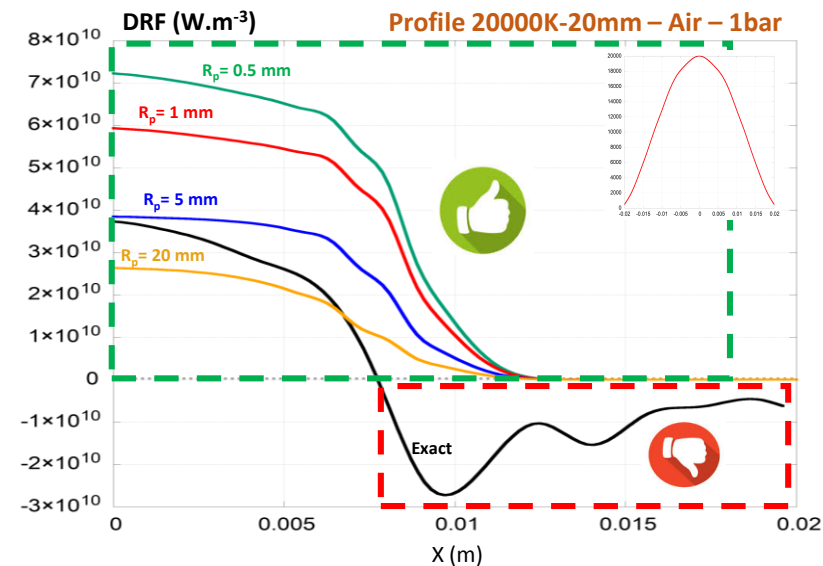
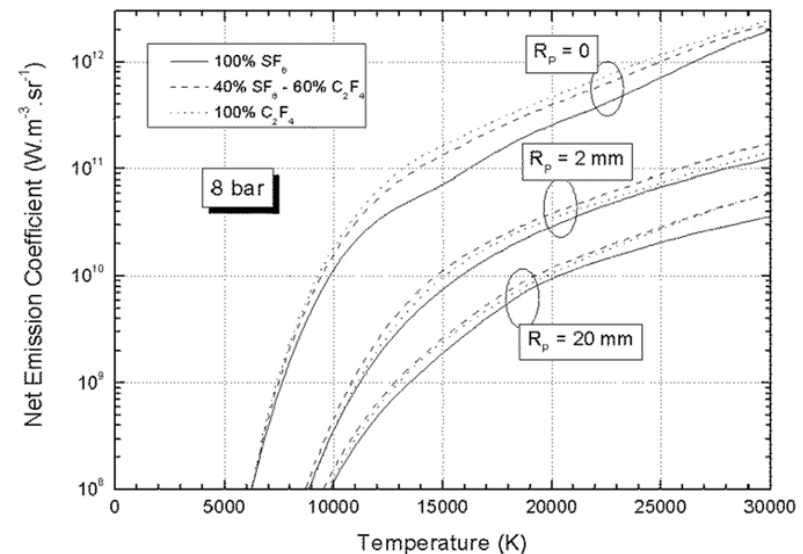
This technique has demonstrated its efficiency to model radiations emitted by central hot regions of the arc.



# The Radiative Transfer Equation (RTE) - The Net Emission Coefficient (NEC)

If temperature ↗	NEC ↗
If pressure* ↗	NEC ↗
If plasma's size $R_p$ ↗	NEC ↘
If metallic vapors ↗	NEC ↗
If organic vapors ↗	NEC ↗↘
If escape factor ↗	NEC ↗

\* Limited by Black body radiation



## How to choose the value of $R_p$ ?

### Proposition of M. Fang & A. Gleizes

$R_p$  roughly corresponds to the radius of the hot region of the plasma, which is an expression not very precise, but a rather good estimation is the **distance from the axis** where the temperature has a value of **about 80% of the axis temperature**.

$$R_p = r (T=80\%T_{max})$$

Y Cressault, A Gleizes and G Riquel, « Properties of air-aluminum thermal plasmas », J. Phys. D: Appl. Phys. 45 (2012) 265202 (12pp)

### Proposition of L. Fulcheri

The plasma thickness  $R_p$  which helps better handling peaks in the absorption spectrum, can be fairly **approximated with  $2*r_o$**  ( $r_o$  radius of the cylindrical arc). However, the arc radius  $r_o$  is a function of the pressure, current and the tube radius  $R$ .

$$\frac{2}{r_o^2} \int_0^{r_o} r dr \nabla \cdot \vec{q}_{rad} = \frac{2\pi B_\nu}{r_o} S_{exact}(k_\nu r_o) \Rightarrow r_o \Rightarrow R_p = 2*r_o$$

P. Gueye, Y. Cressault, V. Rohani, and L. Fulcheri, « A simplified model for the determination of current-voltage characteristics of a high pressure hydrogen plasma arc », Journal of Applied Physics 121, 073302 (2017)

### Proposition of N.Kabbaj

To have a good estimation of the radiative losses in the hottest regions, the value of  $R_p$  depends on the maximal temperature, the width of the temperature profile, and the pressure. Nevertheless, different tests on air seems to confirm that  **$R_p=r$  at 90% of  $T_{max}$**  is a good approximation.

$$R_p = r (T=90\%T_{max})$$

N. Kabbaj, « étude du transfert radiatif d'un plasma thermique d'air : Influence des propriétés radiatives dans la modélisation d'un arc libre », PhD Thesis, University of Toulouse (2019)

## Optimization of $R_p$

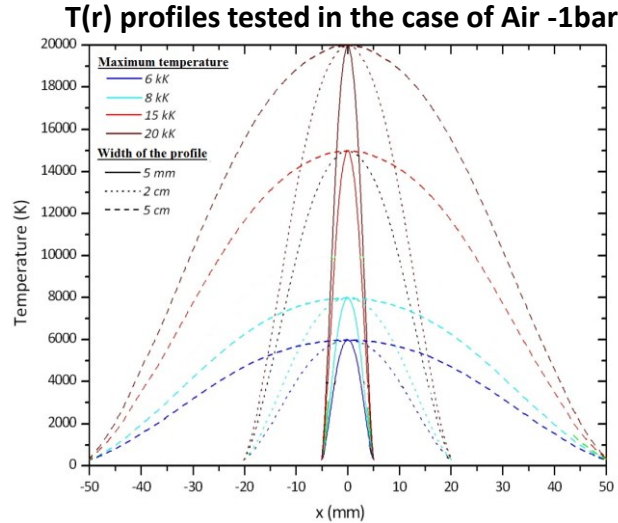
To find the best  $R_p$  to use in modelling

Minimization of

$$F'_{NEC}(R_p) = \frac{|DRF_{exact}(X=0) - DRF_{NEC-Rp}(X=0)|}{DRF_{exact}(X=0)}$$



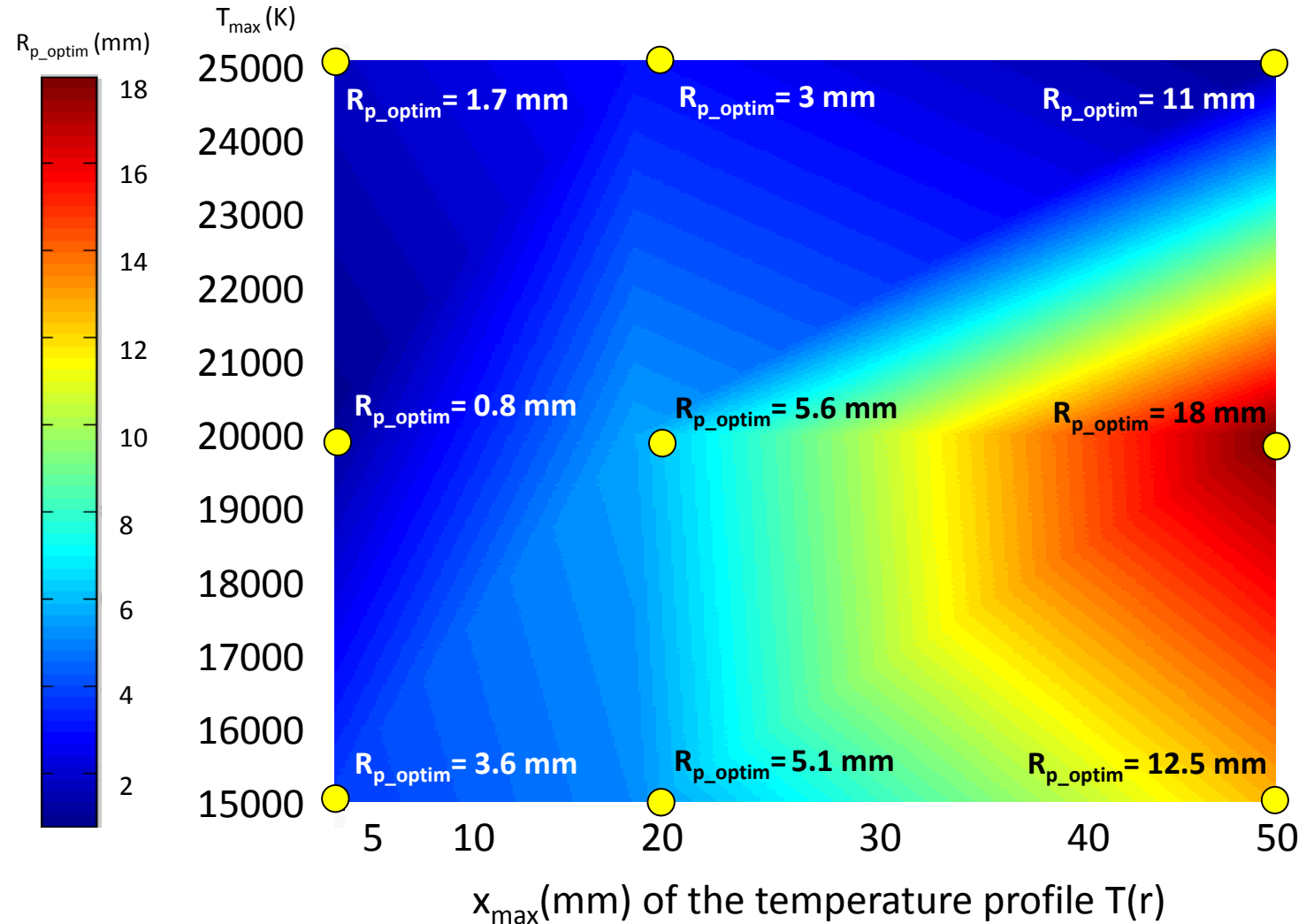
Simplex Nelder Mead algorithm



$T_{max}$ (K)	$r_{max}=5mm$		$r_{max}=20mm$		$r_{max}=50mm$	
	$R_{p\_optim}$ (mm)	% of $T_{max}$	$R_{p\_optim}$ (mm)	% of $T_{max}$	$R_{p\_optim}$ (mm)	% of $T_{max}$
15000	3.6	92	5,1	90	12.5	95
20000	0.8	93	5,6	88	18	81
25000	1.7	91	3	91	11	85

### Conclusions for $R_p$

$R_p = x \sim 90\%$  of  $T_{max}$  is a good choice



## Radiative losses :

Use of spectral simplifications  
to solve the RTE

## Radiative Transfer Equation (RTE)

$$\vec{s} \cdot \vec{\nabla} L_\lambda = K' \cdot L^0_\lambda - K' \cdot L_\lambda$$

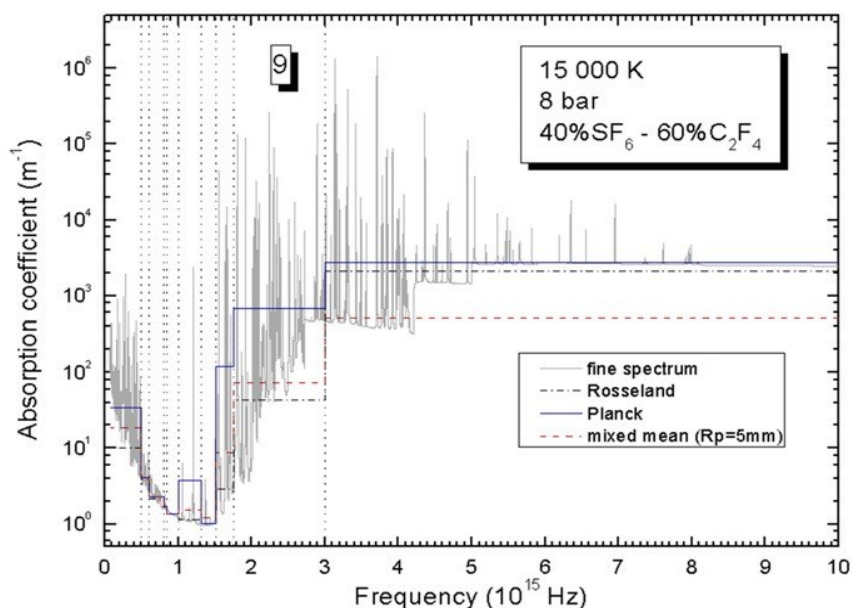
Wavelengths



Too many spectral variations  
**Spectral simplifications**

## The Mean Absorption Coefficients (MACs)

The mean absorption coefficients (MACs) allow an acceptable description of the radiation absorption in the cold regions of the plasma. The latter is a very simplified spectral description based on the splitting of the spectrum into a restricted number of intervals.



Choice of the spectral intervals (SF<sub>6</sub>)

n°	f <sub>1</sub> (10 <sup>15</sup> Hz)	f <sub>2</sub> (10 <sup>15</sup> Hz)
1	0.066	0.200
2	0.200	0.822
3	0.822	1.700
4	1.700	2.074
5	2.074	2.505
6	2.505	4.212
7	4.212	10

H.Z. Randrianandraina, Y. Cressault and A. Gleizes, « Improvements of radiative transfer calculation for SF<sub>6</sub> thermal plasmas », J. Phys. D: Appl. Phys. 44, 19 (2011)

H. Nordborg and A. A. Iordanidis, « Self-consistent radiation based modelling of electric arcs: I. Efficient radiation approximations », J. Phys. D: Appl. Phys. 41 (2008) 135205 (10pp)  
v<sub>10</sub> = {0.0, 1.0, 1.4, 1.77, 2.0, 2.2, 2.5, 3.0, 10.0}

Choice of the spectral intervals (SF<sub>6</sub>-C<sub>2</sub>F<sub>4</sub>)

n°	f <sub>1</sub> (10 <sup>15</sup> Hz)	f <sub>2</sub> (10 <sup>15</sup> Hz)
1	0.066	0.5
2	0.5	0.6
3	0.6	0.8
4	0.8	0.85
5	0.85	1.0
6	1.0	1.31
7	1.31	1.52
8	1.52	1.76
9	1.76	3
10	3	10

C. Ion, Y. Cressault, A. Gleizes and K. Boushara, « Calculation of radiative properties of SF<sub>6</sub>-C<sub>2</sub>F<sub>4</sub> thermal plasmas—application to radiative transfer in high-voltage circuit breakers modelling », J. Phys. D: Appl. Phys. 47 (2014) 013204 (14pp)

Choice of the spectral intervals (CO<sub>2</sub>)

n°	f <sub>1</sub> (10 <sup>15</sup> Hz)	f <sub>2</sub> (10 <sup>15</sup> Hz)
1	0.10	0.50
2	0.50	1.50
3	1.50	2.20
4	2.20	2.72
5	2.72	3.29
6	3.29	8.49
7	8.49	10

S. KOZU, T. FUJINO, T. YOSHINO, T. MORI, RADIATIVE TRANSFER CALCULATION OF CO<sub>2</sub> THERMAL PLASMA USING A HYBRID PLANCK-ROSSELAND MEAN ABSORPTION COEFFICIENT, GD2018 conference, Serbia, 2018

## Classic mean function

$$\bar{\kappa}'([\lambda_i, \lambda_j], T) = \frac{\int_{\lambda_i}^{\lambda_j} \kappa'(\lambda, T) d\lambda}{\int_{\lambda_i}^{\lambda_j} d\lambda}$$

Valid at very low T

## Planck mean function

$$\bar{\kappa}'([\lambda_i, \lambda_j], T) = \frac{\int_{\lambda_i}^{\lambda_j} \kappa'(\lambda, T) \cdot L_{\lambda}^0(T) d\lambda}{\int_{\lambda_i}^{\lambda_j} L_{\lambda}^0(T) \cdot d\lambda}$$

Optically thin  
Overestimation

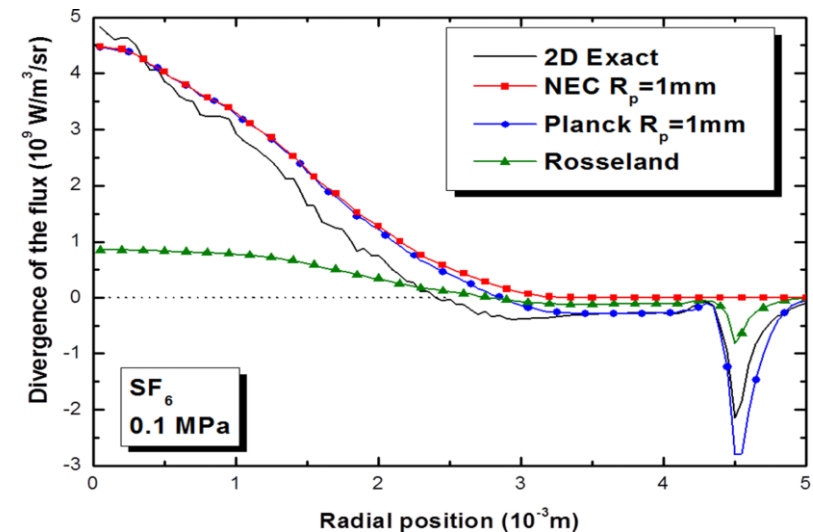
## Planck Modified Mean Function (PMMF)

$$\bar{\kappa}'([\lambda_i, \lambda_j], T, \mathbf{R}) = \frac{\int_{\lambda_i}^{\lambda_j} \kappa'(\lambda, T) \cdot L_{\lambda}^0(T) \cdot \exp(-\kappa'(\lambda, T) \cdot \mathbf{R}) d\lambda}{\int_{\lambda_i}^{\lambda_j} L_{\lambda}^0(T) \cdot d\lambda}$$

## Rosseland mean function

$$\bar{\kappa}'([\lambda_i, \lambda_j], T) = \frac{\int_{\lambda_i}^{\lambda_j} \frac{dL_{\lambda}^0(T)}{dT} \cdot d\lambda}{\int_{\lambda_i}^{\lambda_j} \frac{dL_{\lambda}^0(T)}{dT} \cdot \frac{1}{\kappa'(\lambda, T)} \cdot d\lambda}$$

Optically thick  
Underestimation



How many spectral intervals?  
Which mean function do I use?

### Recent works – different approaches - HVCB

1/ **Use of PMMF** : H. Norborg (SF<sub>6</sub>, 2008), H.Z. Randrianandraina (SF<sub>6</sub>, 2011), by improvement of spectral intervals.

2/ **Mix of Mean functions** : C. Jan (SF<sub>6</sub>-C<sub>2</sub>F<sub>4</sub>, 2013)

3/ **Optimization algorithm** : P. Kloc (Air, 2017), N.Kabbaj (Air, 2018)

4/ **Hybrid Mean function** : H. Norborg (SF<sub>6</sub>, 2018), T. Fujino (CO<sub>2</sub>, 2018), P. Kloc (Air, 2019)

Optimization algorithm : **To find the best unique R (for all spectral interval) or best  $R_i$  for each interval**

Define on each spectral interval a characteristic absorption length  
 $R = [R_{1\text{-optim}}, R_{2\text{-optim}}, R_{3\text{-optim}}, R_{4\text{-optim}}, R_{5\text{-optim}}, R_{n\text{-optim}}]$

**Objectives** ↓

**Simplex Nelder Mead**

X points along the diameter (1D)

Minimization of the errors on radiative quantities

**Minimize**  

$$F'_{MAC-Function}(R) = \frac{\frac{1}{X} \sum_{i=1}^X |F_{exact,i} - F_{CMA,i}(R)|}{\frac{1}{X} \sum_{i=1}^X |F_{exact,i}|}$$

**1- Outgoing Radiative Flux (ORF)**

$R_{1\text{-optim}}$  to  $R_{n\text{-optim}}$

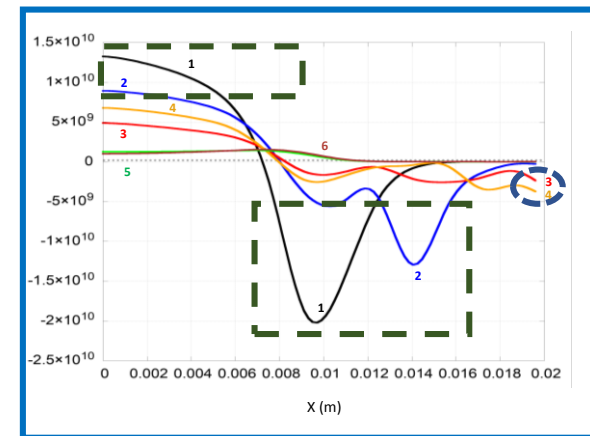
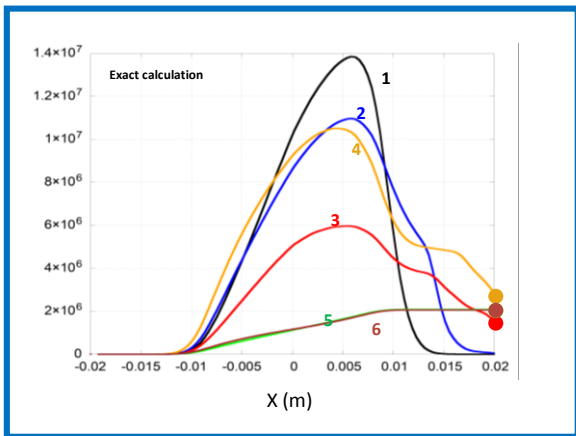
**2- DRF**

$R_{1\text{-optim}}$  to  $R_{n\text{-optim}}$



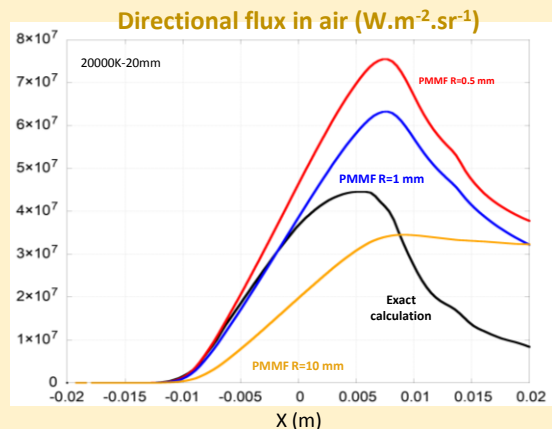
**3- Simultaneously the DRF and the ORF**

$R_{1\text{-optim-DRF}}$  &  $R_{i\text{-optim-DRF}} + R_{j\text{-optim-ORF}}$  to  $R_{6\text{-optim-ORF}}$



Optimization algorithm : **To find the best unique R (for all spectral interval) or best  $R_i$  for each interval**

## 1- Outgoing Radiative Flux (ORF)



$R_1$ -optim to  $R_6$ -optim

Profile	$F'_{MAC-ORF}$ (%)
15000K-5mm	1.2
15000K-20mm	0.08
15000K-50mm	0.09
20000K-5mm	0.62
20000K-20mm	0.61
20000K-50mm	0.04
25000K-5mm	0.6
25000K-20mm	0.0012
25000K-50mm	0.0009

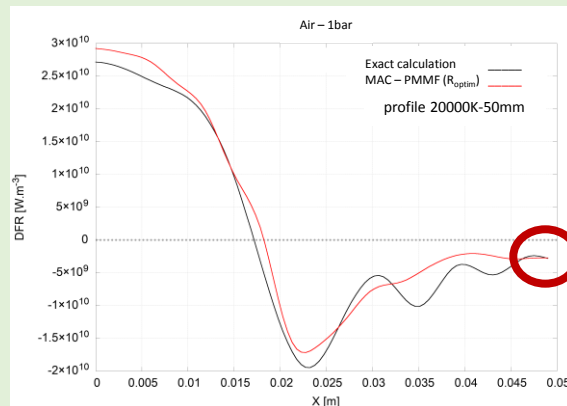
With unique R: 9%

Growth of the error



Error less than 1.5%

## 2- DRF

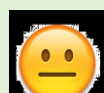


$R_1$ -optim to  $R_6$ -optim

Profile	$F'_{MAC-DRF}$ (%)
15000K-5mm	6
15000K-20mm	7.1
15000K-50mm	8.8
20000K-5mm	9
20000K-20mm	9.5
20000K-50mm	11.4
25000K-5mm	14
25000K-20mm	14.2
25000K-50mm	18

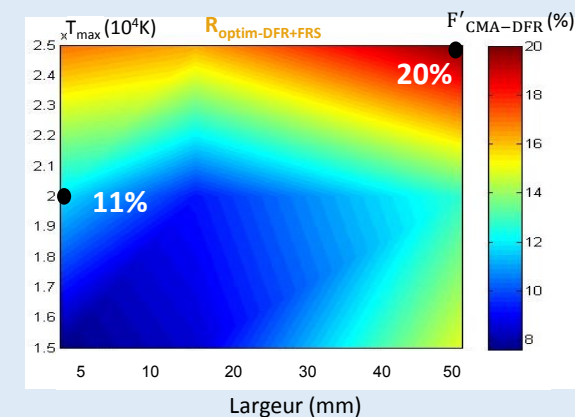
With unique R: 47%

Growth of the error

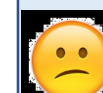


Error between 6-14%

## 3- Simultaneously the DRF and the ORF



Profile	$F'_{MAC-DRF}$ (%)	$F'_{MAC-ORF}$ (%)
15000K-5mm	7.6	3
15000K-20mm	8.5	0.007
15000K-50mm	15	3
20000K-5mm	11.83	0.9
20000K-20mm	9.24	3.6
20000K-50mm	12.8	4
25000K-5mm	17	6.2
25000K-20mm	16.3	0.002
25000K-50mm	20	8



Error between 0.1-20%

# The Radiative Transfer Equation (RTE) - Mean Absorption Coefficients (MACs)

Use of Hybrid Planck-Rosseland (P-R)  $\rightarrow \kappa_{i,Hybrid} = (1 - \gamma)\kappa_{i,Planck} + \gamma\kappa_{i,Rosseland}$

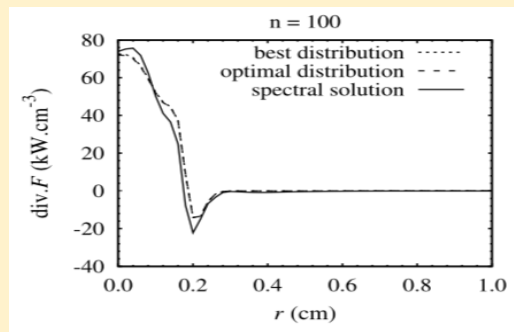
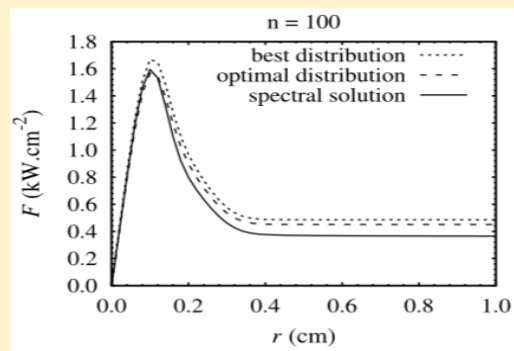
Special treatment for atomic lines  $\rightarrow$

$$\kappa_{\nu,line} = \frac{1}{h} (1 - \exp(-\kappa_{\nu,line}h))$$

Model 1D, 79.714 frequencies,  
7 spectral intervals, profile  $T_{max}=20000K$   
 $2.20 - 2.7210^{15}Hz$

P. Kloc (Air, 0.5-5 bar, 2018)

2 profiles, 3 bands  
optimization function



$H = 2R_p (0.5bar) - 3R_p (5 bar)$   
 $L_1=2.93759 \times 10^{15} Hz, L_2=3.51299 \times 10^{15} Hz$

P. Kloc, V. Aubrecht and M. Bartlova, Numerically optimized band boundaries of Planck mean absorption coefficients in air plasma, Journal of Physics D: Applied Physics, 50, 30, 305201 (2017)

R. Fuchs (SF<sub>6</sub>, 10 bar, 2018)

LTE stabilized arc, cylindrical, SF<sub>6</sub>  
I=100A, 400 pts,  $T_{wall}=300K, r_{wall}=5mm,$   
7 : 0.066, 0.35, 1.54, 2.65, 2.94,  $3.52 \times 10^{15}Hz$

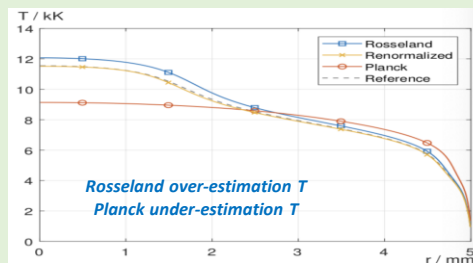
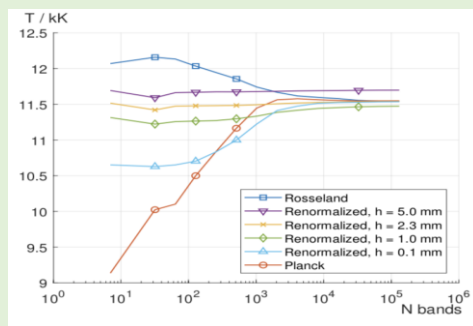


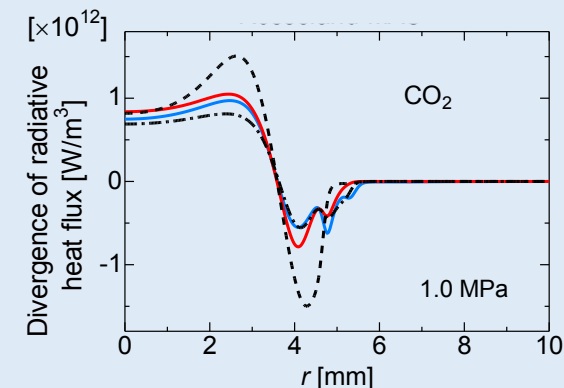
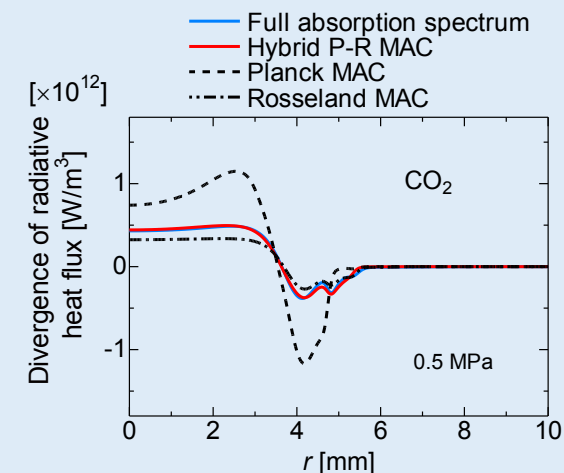
Fig. 1: Temperature profiles for low number of spectral bands.



Planck mean = Rosseland mean if bands > 10<sup>3</sup>  
Re-normalized function is acceptable with  
 $h=2.3mm$

R. FUCHS, H. NORDBORO, SYSTEMATIC INVESTIGATION ON RADIATION MODELING ERRORS OF A WALL-STABILIZED ARC SIMULATIONS, GD2018 conference, Serbia (2018)

T. Fujino (CO<sub>2</sub>, 0.5-1 bar, 2018)



S. Kozu, T. Fujino, T. Yoshino, T. Mori, Proceedings of 22nd International Conference on Gas Discharges and Their Applications, No. A21, pp.127-130 (2018)



# Radiative properties in non LTE

- ① Some works on applications such as atmospheric entry, combustion : *Lamet et al, Riviere et al, Perrin et al*
- ② Recent works 2T numerical modelling (*J.P. Trelles, M.Baeva, M.Benilov, J.Yan, P.Freton* : 2 equations : with  $T_e$  and  $T_g$ )
- ③ Any work on radiative properties for HVCB and RTE equation in 2T (some works on transport properties, compositions)
- ④ First studies in Laplace laboratory with  $SF_6$ ,  $SF_6-C_2F_4$  with first steps : use of the Net Emission Coefficient (NEC) in 2T

## Compositions defined from different assumptions (Mass action law, Kinetic model, Radiative collisional model....)

➡ Different assumptions on the temperatures ( $T_{ex}$ ,  $T_e$ ,  $T_g$ ,  $T_{vib}$ ,  $T_{rot}$ ) and **parameter  $\theta$**

### For the radiation of the continuum (atomic + molecular)

- Recombination ( $T_e$ ) + Bremsstrahlung electron-atom ( $T_e$ )
- Bremsstrahlung electron-ion ( $T_e$ ) + Attachment ( $T_e$ )

$$\epsilon_N^{cont}(\theta, T_e) = \int_0^\infty \epsilon_\lambda^{cont} e^{-\kappa'_{tot} R_p} d\lambda = \int_0^\infty B_\lambda(\lambda, T_e) \kappa'^{cont} e^{-\kappa'_{tot} R_p} d\lambda$$

$$\kappa'^{tot}(\theta, T_e) = \kappa'^{cont}(T_e) + \kappa'^{lines}(T_{ex})$$

### For the radiation of the atomic lines

- Broadenings : Doppler ( $T_g$ ) + Resonance ( $T_{ex}$ ) + Van der Waals ( $T_g$ ) + quadratic Stark ( $T_e$ ) + Griem corrections ( $T_e$  for electrons,  $T_g$  for ions) + quadripolar Stark ( $T_e$ )

$$\epsilon_{\lambda,ul}^A = \frac{he^2}{2\epsilon_0 m_e (\lambda_{ul} + \Delta_{ul})^3} \frac{n_A}{Q_{int}^A} g_l e^{-\beta_{ex} E_{il}^A} f_{lu} V(\lambda - \lambda_{ul} - \Delta_{ul})$$

$$\kappa'_{ul}^A = \frac{e^2 (\lambda_{ul} + \Delta_{ul})^2}{4\epsilon_0 m_e c^2} f_{lu} \frac{n_A}{Q_{int}^A} g_l e^{-\beta_{ex} E_{il}^A} \left[ e^{\beta_{ex} \frac{hc}{(\lambda_{ul} + \Delta_{ul})}} - 1 \right] V(\lambda - \lambda_{ul} - \Delta_{ul})$$

## The Net Emission Coefficient (NEC) - LTE



NEC gives a good estimation of radiation in the hottest regions (if high temperatures and low temperature gradients <20% in the first mm)  
NEC gives information on the influence of T, P, metallic and/or organic vapors, on self-absorption ( $R_p$ )  
NEC considers all radiative processes / the spectral dependence, NEC is very simple to implement in MHD models



NEC does not describe the radiative flux, NEC does not consider the absorption in intermediate/cold regions  
NEC is limited by the Blackbody radiation,  $R_p$  must be well chosen in MHD model

## The Mean Absorption Coefficients (MACs) - LTE



MACs can give a good estimation of radiation in the intermediate regions by considering the absorption  
MACs allow the calculation of the radiative & divergence of the radiative flux, MACs considers all radiative processes



MACs efficiency depends on the mean functions used, MACs using Modified Planck Function need to find the good  $R_p$   
Its is very difficult to estimate correctly the radiative flux and the divergence of the radiative flux with the same MACs

## Future works – The radiative properties for Thermal Plasmas

**NEC : No new developments** - Elaboration of new databanks (new gases or mixtures), Validity at very high pressure (non ideal gas) ? Optimization to find the best  $R_p$ . Validation is necessary by experimental measurements (Laplace group did it on Air and ArH<sub>2</sub> mixtures on spectral intervals and atomic lines).

**MACs : calculations to perform** - must be carefully performed to describe the increase of pressure in HVCB (absorption of radiation / ablation of materials), MACs with hybrid Planck + Rosseland seems to be a good solution (at 1atm or close to 1atm). And for very high P (>5bar) ? MACs for complex mixtures (SF<sub>6</sub>/C<sub>2</sub>F<sub>4</sub>...) ? RTE with a non-symmetrical temperature profile ? Validation is necessary by experiment measurements (Laplace group and Siemens did it by comparing the increase of pressure in SF<sub>6</sub>/C<sub>2</sub>F<sub>4</sub> HVCB experiments-modelling)

**2T properties** : not necessary to have good accuracy because we have a low radiation in these regions.

No relation between absorption and emission!!! To use Kirchhoff law is questionable! Kirchhoff's law ( $T_e$  or  $T_{ex}$ ):  $\epsilon \rightarrow \kappa'$

NEC is a first approximation at low temperature. Not so good or not so bad??? What about MACs at 2T ?

Necessary to develop a **CR model by levels** : more accurate but it is a very BIG work

