ÉTUDE EXPÉRIMENTALE
ET SIMULATIONS NUMÉRIQUES
DE L’INTERACTION ENTRE UN RAYONNEMENT
MICROONDE DE FRÉQUENCE VARIABLE
ET UN ANALOGUE DE SUIE DE PROPANE
RÉALISÉ PAR STÉRÉOPHOTOLITHOGRAPHIE

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propane soot 3D morphology description by high resolution SEM tomography [G. Okyay et al, J. Aerosol Science 93 (2016), 63-79]

tomogram – 11 high resolution SEM micrographs – tilt angles: from -50° to +50°

SEM tomography

reconstructed 3D geometry

TEM image

\[ d_{\text{monomer}} \approx 20 \text{ nm} \]
numerical generation of representative soot aggregates

fractal analysis of the tomographed objects

→ value of the fractal prefactor \( k_f \)

→ value of a penetration coefficient of the primary particles:

\( Cp \approx 0.5 \) for both tomographed soot aggregates

\( C_p = 0 \)

\( C_p = 0.5 \)

\( C_p \approx 1 \)

\( N_p = 940 \quad d_p = 28 \text{ nm} \)

\( N_p = 1250 \quad d_p = 28 \text{ nm} \)
calculation of the radiative properties of complex shaped objects by the Discrete Dipole Approximation (DDA)

\[ P_j(t) = \alpha_j \mathbf{E}_{\text{loc}}(r_j, t) \]

\[ = \alpha_j \left\{ \mathbf{E}_{\text{inc}}(r_j, t) + \sum_{1 \leq k \leq N \atop k \neq j} \left( \mathbf{E} \text{ produced at location } r_j \text{ by } P_k(t) \text{ located at } r_k \right) \right\} \]

\[ = \alpha_j \left\{ E_0 \mathbf{e} \exp(i(K \mathbf{u} \cdot r_j - \omega t)) + \sum_{1 \leq k \leq N \atop k \neq j} \left[ A(r_j - r_k) \right] \cdot \mathbf{P}_k(t) \right\} \]

\[ \frac{\Pi_j}{\alpha_j} - \sum_{1 \leq k \leq N \atop k \neq j} \left[ A(r_j - r_k) \right] \cdot \mathbf{P}_k = E_0 \mathbf{e} \exp(i K \mathbf{u} \cdot r_j) \text{ for all } j = 1, 2, \ldots N \]

\[ \Pi_j \left( \text{geometry } (r_k), \text{ materials } (\alpha_k), \lambda, \mathbf{u}, \mathbf{e} \right), \ j = 1, 2, \ldots N \]

interaction cross-sections \( C_{ext, abs, sca}^{P or NP}(\mathbf{u}, \mathbf{e}) \) and scattering phase function \( \Phi_{P or NP}(\mathbf{u}, \mathbf{u}', \mathbf{e}) \)
DDA calculation of the radiative properties of the 3 soot aggregates
[ G. Okyay, PhD thesis, CentraleSupélec, April 2016 ]

excellent representativity of the virtual (DLCCA) aggregate with overlapping particles
radiative properties significantly altered when particle overlapping (≈ sintering) is taken into account
validation of the DDA calculations on an enlarged (x 66667) soot aggregate – collaboration CETHIL + EM2C + Institut Fresnel

microwave analogy:

1/ fabrication by stereophotolithography (CTTM, Le Mans, France) of an enlargement (x 66667 : 500 nm $\rightarrow$ 3 cm) of this soot aggregate made of a non absorbing resin

2/ microwave experiments (wavelengths x 66667 : $\mu$m $\rightarrow$ dm) (CCRM, Marseille, France)

spatial sampling (voxelization) of this enlarged soot aggregate (7494 cubes of edge $\approx$ 690 $\mu$m) for DDA calculations ($m = 1.72 + j \times 2.47 \times 10^{-2}$ independent of $\lambda$)
validation of the DDA calculations on an enlarged \((x \times 66667)\) soot aggregate – collaboration CETHIL + EM2C + Institut Fresnel

\(\approx 500 \text{ nm}\)

scale factor \(k = 66667\)

\(0.25 \mu m \leq \lambda \leq 2.25 \mu m\)

34 mm

analog fabrication by stereophotolithography (CTTM, Le Mans, France)

analog made of a non absorbing resin

16.7 mm \(\leq \lambda \leq 150\) mm

2 GHz \(\leq \nu \leq 18\) GHz

spatial sampling (voxelization) of this enlarged soot aggregate (7494 cubes of edge \(\approx 690 \mu m\))

for DDA calculations

\((m = 1.72 + j \times 2.47 \times 10^{-2}\) independent of \(\lambda)\)
Microwave anechoic chamber of CCRM (Marseille, France)

microwave source:
- linearly polarized monochromatic frequency tunable radiation
- (4 GHz ≤ ν ≤ 18 GHz)
- (7.5 cm ≥ λ ≥ 1.67 cm)

microwave detector:
- collects the local E field (amplitude and phase)

target
Microwave anechoic chamber of CCRM (Marseille, France)

Microwave source
linearly polarized monochromatic frequency tunable radiation
(4 GHz ≤ ν ≤ 18 GHz)
(7.5 cm ≥ λ ≥ 1.67 cm)

Microwave detector collects the local E field (amplitude and phase)

Target
Receiver plane
validation of the DDA calculations on the enlarged soot aggregate
vertically polarized incident radiation
extinction cross section spectra of the enlarged soot aggregate
measured (CCRM anechoic chamber) and calculated (DDA)
for 4 aggregate orientations:

(4 GHz ≤ ν ≤ 18 GHz corresponds to 7.5 cm ≥ λ ≥ 1.67 cm)
validation of the DDA calculations on the enlarged soot aggregate

frequency $\nu = 16$ GHz – vertical polarization – orientation $= 0^\circ$ (top) and $90^\circ$ (bottom)
calculation of the scattered field of complex shaped objects by the Volume Integral Method resolved by the Method of Moments (MoM)

\[
\vec{E}_s(r) = \int_{\Omega} \vec{G}(r, r') \chi(r') \vec{E}(r') dr'
\]

\[
\vec{E}(r) = \vec{E}_i(r) + \int_{\Omega} \vec{G}(r, r') \chi(r') \vec{E}(r') dr'
\]

with \( \chi(r') = k^2 (r') - k_o^2 \)

Resolution: **Method of Moments** (MoM)

with Bi-Conjugated Gradient Stabilized-FFT method

- using the Toeplitz properties of the free space Green function

  involving only a 1D-FFT

  - computation complexity: \( O(N \log(N)) \) (\( N \) : number of cells)
  - memory requirement: \( O(N) \)

[ O. Merchiers et al, Optics Express 18 (2010), 2056-2075 ]
validation of the MoM calculations on the enlarged soot aggregate

vertically polarized incident radiation

extinction cross section spectra of the enlarged soot aggregate

measured (CCRM anechoic chamber) and calculated (MoM)

for 4 aggregate orientations:

\[
\begin{align*}
C_{\text{ext}} & = 0.2 \times 10^{-3} \\
\text{frequency (GHz)} & = 4 \leq \nu \leq 18 \\
\text{corresponds to} & \quad 7.5 \text{ cm} \geq \lambda \geq 1.67 \text{ cm}
\end{align*}
\]
Vertically polarized incident radiation

Target discretization:
- Cubic cells
- Edge \( a \approx 690 \mu m \)
- Frequency range: \( 2 \text{ GHz} \leq \nu \leq 18 \text{ GHz} \)

\[ a \leq \lambda/24 \]

\( R = \text{radius of the volume equivalent sphere} = 8.1 \text{ mm} \)
$C_{\text{ext}}$ spectra for 3 initial (morphology) voxelizations of the object

target discretization:
- cubic cells
- edge $a$ variable:
  - $a_1 \approx 690 \, \mu\text{m} \leq \lambda/24$
  - $a_2 = 2a_1 \leq \lambda/12$
  - $a_4 = 4a_1 \leq \lambda/6$

measurement
- DDA (----) - $a_1 \leq \lambda/24$
- MoM (- - -) - $a_1 \leq \lambda/24$
- DDA (----) - $a_2 \leq \lambda/12$
- MoM (- - -) - $a_2 \leq \lambda/12$
- DDA (----) - $a_4 \leq \lambda/6$
- MoM (- - -) - $a_4 \leq \lambda/6$
$C_{\text{ext}}$ spectra after subvoxelization of the 3 initial voxelizations

target discretization:
cubic cells

dge $a$ approximately identical for the 3 discretizations

$a \approx 690 \, \mu m \leq \lambda/24$

measurement

DDA (----) - $a \leq \lambda/24$

MoM (---) - $a \leq \lambda/24$
numerical errors of DDA and MoM due to insufficient discretization of a given morphology

insufficient discretizations:

- \( a \leq \lambda/12 \)
- \( a \leq \lambda/6 \)

improved discretizations:

- \( a \leq \lambda/24 \)
- \( a \leq \lambda/24 \)

**Measurement**

- DDA (----) - \( a \leq \lambda/12 \)
- MoM (---) - \( a \leq \lambda/12 \)
- DDA (----) - \( a \leq \lambda/6 \)
- MoM (---) - \( a \leq \lambda/6 \)
summary

- excellent agreement between the measured $C_{\text{ext}}$ and $E_{\text{sca}}$ amplitude and phase spectra and their counterparts issued from DDA and MoM calculations
  - validation of the experiments and of the calculations
- differences between experiments and simulations essentially due to differences between $V$(aggregate of experiments) and $V$(discretized aggregates in simulations)
- the slight differences between DDA and MoM results could be attributed to:
  - the polarizability prescription (CMRR) retained in the DDA calculations
  - the spatial periodicity implicitly assumed in the MoM calculations (FFT)
- the impact of the finesse of the initial (morphology) discretization appears to be relatively weak, provided that a subsequent subdiscretization is applied to this initial discretization in order to satisfy the conditions of validity of DDA and MoM calculations: $|m|Ka < 1$

perspectives

- try to understand the differences between DDA and MoM results
- validate the conclusions issued from the calculations with experiments performed on aggregates of different spatial discretizations
- work with a bigger aggregate presenting more pronounced morphological anisotropy
- introduce absorption in the resin