Optical diagnostics in fluid mechanics Metrology of particles

Part 2: Theories

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Theories of light scattering

Approximate models and theories

- Geometric optics \rightarrow VCRM
- Diffraction
- Ray theory of waves
- Rayleigh theory
- •••••

General Rigorous theories

- Lorenz-Mie theory
- Generalized Lorenz-Mie theory
- Numerical methods
 - T-matrix, DDA
 - MoM, FTDT, FEM, ...





Geometric optics

What is it used for ?

Imaging in daily life:

- Image by reflection: mirror in car, water surface, summer route ...
- Image by refraction: fish, stick in water, mirage in the nature ...

> Optical instruments:

- Camera, telescope, microscope, ...
- Industrial measurement systems,
- Optical fiber for telecommunication

Scientific research:

- Fluid mechanics: PIV, holography, LDV, PDA,
- Measurement of temperature, size distribution, ...
- Biological imaging, …



Advantages:

- Simple
- Object of arbitrary shape



Geometric optics

Condition and simple applications

Conditions :

 $\lambda \ll l$

The wave length λ is much longer than the dimension of the object **I**.

1. Straight propagation in a homogeneous medium



























Total reflection - applications







 n_1

 n_2 n_3 n_4

...

 $n_{\rm p}$

Relation of amplitudes and intensities

Fresnel formulas – relation between the amplitudes of the reflected/refracted and incident waves









В

Geometric optics – propagation of light in a medium

optical path, phase and intensity

Propagation of light in a medium:
Optical path:

$$\tau(AB) = \int_{A}^{B} m(s) ds$$

A $d\tau = m ds$
Complex refractive index:
 $\tilde{m} = m_r - im_i$
• Phase difference : $\Delta \varphi(AB) = k\tau_r = km_r \Delta S$
• Absorption: $I(B) = I(A) \exp(-2k\tau_r) = I(A) \exp(-2km_r \Delta S)$

• If *m* is constant: $\Delta \phi = km_r \Delta S$

$$I = I_0 \exp(-2km_i \Delta S)$$





Can GO be applied to light scattering ?

<u>YES</u> to the simple particles:

- Homogeneous sphere,
- Homogeneous circular cylinder

Possible for objects of complex shape:

- Pure ray model, precision is very limited
- Ray model + electromagnetic integration, much better
- Ray model + wave properties → <u>Vectorial Complex Ray Model</u>

→ New concept, very precise and easy to use.





Reflection and refraction in a particle

Light scattering by a sphere:

• Intensity :



 $\theta_p = 2\tau - 2p\tau'$





Reflection and refraction in a particle

>Phases:

• Phase difference <u>due to the difference of the op</u>tical paths :

$$\Delta \phi = \frac{2\pi d}{\lambda} \left(\sin \tau - pm \sin \tau' \right)$$

- Jump of phase due to reflection on the surface and the focal lines.
 -) Reflection: phase of the complex number: $r_{X,}$
 - 2) Focal lines: phase jump $\pi/2$ at each focal line.
- Divergence factor :

$$D_{p} = \frac{\cos \theta_{i} \sin \tau}{\sin \theta_{p} \left| \frac{d\theta_{p}}{d\tau} \right|}$$

$$I_{s,p} = \frac{I_0 \varepsilon_X dS_i}{dS_s} = \frac{I_0 \varepsilon_X a^2 \cos \tau \sin \tau d\tau d\varphi}{r^2 \sin \theta_p d\theta_p d\varphi} = \frac{a^2}{r^2} I_0 \varepsilon_X D_p$$



These equations are enough to calculate the intensity of each order and the total field.

$$\widetilde{A}_{s,t} = \sum_{p=0}^{N} \sqrt{I_{s,p}} e^{-i\Delta\phi_p}$$



Scattering diagram according to geometrical optics







Scattering diagram of a water droplet: $a=50\mu m$, $\lambda=0.6328$, m=1.333

















Comparison with rigorous theory

A homogeneous infinite cylinder



Preliminary conclusions

- By taking into account correctly the interferences, the Ray model can predict the scattering diagram in ALL directions.
- > It can be applied to the scattering of **any shaped beam**.
- > It works also for a circular infinite cylinder.

Limitations

NOT appropriate for a spheroid or an ellipsoid NO for any irregular shaped particles.

The key problem is **the divergence factor**.

How to improve the model?







Geometric optics > VCRM

Possible candidate?

- ★ Rigorous theories: the particle shape must correspond to a coordinates system
- * Numerical methods: size limited, very time communing
- ✓ Ray models: precision to be improved

Key problem: lack of wave properties

Our strategy: Extension of ray model

- Inclusion of wave front curvature
- Interference between all the rays.
- Diffraction.

Vectorial Complex Ray Model



Divergence/ Convergence Phase in focal lines





For details:

Vectorial Complex Ray Model

Geometrical optics + wave form

- Vectorial Complex Ray Model new
 - **5 properties of a ray:**

mportant

Classical optics



Advantages:

- Objects of any shape with smooth surface,
- Incident wave of any form,
- Sufficiently precise scattering in all directions,
- All scattering properties of the objet.





Essential of VCRM





Special case of the wave front equation

The rays remain in the same plane -a main direction of the wave front and the particle surface:

- Spherical particle
- Infinite cylinder at normal incidence
- Ellipsoidal particle in the symmetric plane.
- Curvature matrix:

Wave front equation:

$$\frac{k_n'^2}{k'R_1'} = \frac{k_n^2}{kR_1} + \frac{k_n' - k_n}{\rho_1}$$
$$\frac{k'}{R_2'} = \frac{k}{R_2} + \frac{k_n' - k_n}{\rho_2}$$

















All expressed in wave vector components.



Vectorial Complex Ray Model Available at www.amocops.eu

VCRMEII2D : Vectorial Complex Ray Model (VCRM) for Scattering of plane wave by an Elliptical particle in the 2D plane

1. Module for ray tracing







VCRMEII2D : Vectorial Complex Ray Model (VCRM) for Scattering of plane wave by an Elliptical particle in the 2D plane

2. Module for scattering diagrams







Toward the Ray theory of wave

VCRM can predict much better Airy structure than the Airy theory and can be applied directly to non-spherical particle.







Scattering angle, θ

64

 $\theta = 152.7^{\circ}$ $\theta = 153.9^{\circ}$

Normalized scattering intensity [-]

06

0'4

0'2

UNIVERSITÉ



Comparison of VCRM and experimental normalized equatorial scattering diagrams for the droplets of 3 different aspect ratios. From (a) to (c), the droplet's aspect ratio *b/a* increases and refractive index decreases when the implitude of the acoustic field is reduced.



Caustics of GO to be corrected !

II-31











Application to Characterization of non-spherical droplets



(a) Principal radii measured with the rainbow refractometer and imaging system and (b) corresponding evolution of the droplet refractive index during the course of the experiment.





Phenomena of diffraction

The diffraction is the behavior of waves when they encounter an obstacle.

The phenomenon of diffraction is manifested when

- the dimension of the object is of the order of the wavelength,
- there is a brutal variation of the density / amplitude of the wave.



A wave diffracts around an obstacle



Diffraction by a double slit.



Diffraction effect in a rainbow.





Theory of diffraction

Principle of Huygens-Fresnel

(1) The contribution of Huygens (1678)

The wave of light propagates step. Each surface element reached by it behaves as a secondary source that emits spherical wavelets. The new *wavefront is the envelop* of the wavelets and the amplitude of each wavelet is proportional to the size of the element.

(2) The contribution of Fresnel (1818)

The *complex amplitude* of the wave at one point is the *sum of the complex amplitudes* of all the secondary sources at that point. All these waves interfere to form the wave at the considered point.

$$\underline{\psi}(P) = \sum_{i} \underline{\psi}_{i}(M_{i}) Q_{i} \frac{\exp(ikr_{i})}{r_{i}} \Delta S_{i} \qquad \underline{\psi}(P) = \int_{S} \underline{\psi}_{0}(M) Q \frac{\exp(ikr)}{r} \mathrm{d}S$$









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Theory of diffraction

Let
$$\vec{R} = \vec{OM}, \vec{\rho} = \vec{OP}, \vec{r} = \vec{PM}$$

 $r \cong R + \frac{x^2 + y^2}{2R} - \frac{\xi x + \eta y}{R}$
 $\psi(M) = Ke^{ikR} \iint_{S} \psi(P) e^{-ik(\xi x + \eta y)/R} e^{ik(x^2 + y^2)/2R} dS$

Fresnel diffraction (*R* is small): $\psi(M) = Ke^{ikR} \iint_{S} \psi(P)e^{ik(x^2 + y^2)/2R} dS$

Fraunhofer diffraction ($R \rightarrow$ infinity):

$$\begin{split} \psi(\mathbf{M}) &= \mathrm{K}\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}} \iint_{\mathbf{S}} \psi(\mathbf{P}) \; \mathrm{e}^{-\mathrm{i}\mathbf{k}(\alpha x + \beta y)} \mathrm{d}\mathbf{S} \\ \alpha &= \frac{\xi}{\mathbf{R}} = \cos\zeta \mathrm{sin}\theta \; ; \; \beta = \frac{\eta}{\mathbf{R}} = \mathrm{sin}\zeta \; ; \; \gamma = \cos\zeta \mathrm{cos}\theta \end{split}$$





z

Diffraction

Applications

Diffraction by circular disk (sphere): A *circular hole* of radius *r* :

 $x = \rho \cos \phi, y = \rho \sin \phi, dS = dxdy = \rho d\rho dx$

Be cause of the revolution symmetry we can place in the plane of the disk with the origin at the center:

$$a = \sin \theta$$
, $\beta = 0$

 $I = I_0 \left| \frac{J_1(\kappa \sin \theta)}{\kappa \sin \theta} \right|^2$

 $\kappa = 2\pi r/\lambda$

$$\Psi(\alpha,\beta) = C \iint e^{-ik(\alpha x + \beta y)} dx dy = C \int_{0}^{2\pi} \int_{0}^{d} e^{-ik\rho\sin\theta\cos\varphi} \rho d\rho d\varphi = C \frac{J_{1}(\kappa\sin\theta)}{\kappa\sin\theta}$$

$$I = I_{0} \left[\frac{J_{1}(\kappa\sin\theta)}{\kappa\sin\theta} \right]^{2}$$

$$\kappa = 2\pi r/\lambda$$



Applications

Rayleigh criterion:

The first minimum of $J_1(x)$ is located at x=3.832, i.e.:

$$\theta = \frac{1.22\lambda}{D}$$





So it is interesting to have an large opening for a better resolution (telescope, camera, ...)





Diffraction and Interference

Applications



Course M2 EFE – Rouen University

VCRM + Phys. Opt. -> Reay theory of waves





VCRM + Phys. Opt. -> Reay theory of waves

Physical optics

Recall of Airy theory (1838)



$$u = \frac{hv^3}{3a^2}$$
 with $h = \frac{(p^2 - 1)^2}{p^2} \frac{(p^2 - m^2)^{1/2}}{(m^2 - 1)^{3/2}}$

Sir George Airy (1801-1892)



$$e^{-ikv(\theta-\theta_0)+ikhv^3/3a^2} dv$$

- $\begin{bmatrix} G.O. \\ Airy theory \\ \theta_{go}(m) \\ \theta \end{bmatrix}$
- The version of van de Hulst (1957) permits to predict the profile,
- But the absolute or relative intensity?



Ray theory of waves

Physical optics

- Reexamination of Airy theory
 - » Some typical results in the literature:
 - » Tricker: in the book "Introduction to meteorological optics" 1970

$A \sim \sqrt{a/\lambda}$

» Nussenzveig: JOSA 1979 :

 $A \sim (a/\lambda)^{7/6}$

- » Hovenac & Lock: JOSA A 1992
- » R. Lee: Appl. Opt. 1998

20 March 1998 / Vol. 37, No. 9 / APPLIED OPTICS 1507
 Airy & Mie For a given λ, r, and range of θ, the two theories can yield quite different intensity maxima, so must normalize one theory's results in order to compare them with the other's.

Perpendicular polarization





Perpendicular polarization Nussenzveig PRL (1974), JOSA A (1979) Airy fails for pparallel polarization!!





Ray theory of waves

Physical optics

Airy theory in RTW to remove the two approximations

» Phase:
$$\Delta \Phi = \Phi(Q) - \Phi(C) - k \overline{PR}$$

with $\overline{OD} = r_0 \cdot \hat{k}_{r\perp}$
 $\overline{OR} = r \cdot \hat{k}_{\perp}$
 $\overline{OP} = \frac{\overline{OR}}{\hat{k}_r \cdot \hat{k}} = \frac{\overline{OR}}{\hat{k}_{r\perp} \cdot \hat{k}_{\perp}}$
 $\overline{PR} = \overline{OP}(\hat{k} \cdot \hat{k}_{r\perp})$
 $r = \overline{OP}$

» Amplitude:
$$A_P = A_Q \frac{\kappa'_{GQ}}{\kappa_{GP}}$$

 κ_{GX} and κ'_{GX} are the Gaussian curvatures at point X before/after interaction.

Conclusions:

- Both phase and amplitude are calculated **numerically, so** *rigorously*,
- No any hypothesis,
- Same method for **non-spherical particle**.

Ray theory of waves

Physical optics

• Airy theory in RTW – Validation of the results:

Comparison of the total intensities calculated by four methods

perpendicular polarization

parallel polarization

The results of Ray Theory of Waves (green curves) are in very good agreement with Debye (black curves).

Application of RTW

Rayleigh theory

Static field of a dipole

Electric fields

- Two charges +q et q
- Distance b/t them: d
- Dipole moment : *p*=*qd*

$$\Phi_{dipôle} = \frac{q}{4\pi\varepsilon_{ext}} \left(\frac{1}{r_{+}} - \frac{1}{r_{-}}\right)$$
$$\approx \frac{p}{4\pi\varepsilon_{ext}} r^{2} \cos\theta$$

$$\frac{1}{r_{\pm}} \approx \frac{1}{r \mp \frac{d}{2} \cos \theta} \approx \frac{1}{r} \left(1 \pm \frac{d}{2r} \cos \theta \right)$$

Rayleigh theory

Field scattered by an induced dipole

Electrostatic approximation

Conditions:

- 1. Electric field
 - static
 - uniform
- 2. Size of the particle: $l < < \lambda$

Potential of the induced field:

$$\varphi_{ext} = \frac{a_{\cdot}^{3}}{r^{2}} \frac{\varepsilon_{i} - \varepsilon_{ext}}{\varepsilon_{i} + 2\varepsilon_{ext}} E_{0} \cos \theta$$

"Scattered" field:

$$\vec{E} = \frac{4\pi_{\cdot}^2}{r\lambda^2} a^3 \left(\frac{\varepsilon_i - \varepsilon_{ext}}{\varepsilon_i + 2\varepsilon_{ext}}\right) E_0 \sin\theta \,\vec{e}_{\theta}$$

$$d \ll \lambda,$$

 $Q_{ext} = \frac{8}{3} \left(\frac{\pi d}{\lambda}\right)^4 \operatorname{Re}\left(\frac{m^2 - 1}{m^2 + 2}\right)$

Rayleigh theory

Field scattered by an induced dipole

Scattering diagram

Perpendicular polarization

Elements of scattering matrix:

$$S_1 = -\frac{ik^3\alpha}{4\pi}$$

Parallel polarization

Lorenz-Mie Theory - LMT

Conditions and principle

Conditions:

- 1. Incident plane wave
- 2. Particle :
 - Spherical
 - Homogeneous or central stratified
 - Isotropic

Electromagnetic field:

 $E_{n} = A_{n} R_{n}(\mathbf{r}) \Theta(\theta) \Phi(\phi)$ $H_{n} = B_{n} R_{n}(\mathbf{r}) \Theta(\theta) \Phi(\phi)$

Boundary conditions :

$$\begin{split} E_{i,\theta} + E_{s,\theta} &= E_{e,\theta} \\ H_{i,\theta} + H_{s,\theta} &= H_{e,\theta} \end{split}$$

Lorenz-Mie Theory - LMT

Conditions and principle

Incident wave:

$$\begin{pmatrix} U_{TM}^{i} \\ U_{TE}^{i} \end{pmatrix} = \frac{1}{k^{2}} \sum_{n=1}^{\infty} \frac{1}{i^{n+1}} \frac{2n+1}{n(n+1)} \psi_{n}(kr) P_{n}^{1}(\cos\theta) \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix}$$

Lorenz-Mie Theory - LMT

Physical quantities

Scattered intensities:

 $I_{\perp}(\theta) = |S_1|^2$ $I_{\parallel}(\theta) = |S_2|^2$

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_n \pi_n(\cos\theta) + i b_n \tau_n(\cos\theta) \right]$$
$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_n \tau_n(\cos\theta) + i b_n \pi_n(\cos\theta) \right]$$

Efficiency sections : $C_{ext} = C_{sca} + C_{abs}$

$$C_{sca} = \frac{\lambda^2}{2\pi} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2)$$
$$C_{ext} = \frac{\lambda^2}{2\pi} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}(a_n + b_n)$$

Radiation pressure :

$$C_{x} = C_{y} = 0$$

$$C_{pr,z} = \frac{\lambda^{2}}{2\pi} \operatorname{Re}\left[\sum_{n=1}^{\infty} (2n+1)\frac{(a_{n}+b_{n})}{2} - \frac{2n+1}{n(n+1)}a_{n}b_{n}^{*} - \frac{n(n+2)}{n+1}(a_{n}a_{n+1}^{*} + b_{n}b_{n+1}^{*})\right]$$

Generalized Lorenz-Mie Theory - GLMT

Conditions and principle

Conditions:

- 1. Incident wave: *any shape*
- 2. Particle :
 - Spherical
 - Homogeneous or centrally stratified
 - Isotropic

Particularities:

- 1. When the object is big, the illumination is not uniform,
- 2. The incident wave is described by two series of coefficients :

$$g_{n,TE}^m$$

 ∞ m=+n

 $\rightarrow \Sigma \Sigma$

 $\underline{n=1} \qquad \underline{n=1} \ \underline{m=-n}$

 $a_n \rightarrow a_n g_{n,TM}^m$

 $b_n \to b_n g_{n,TE}^m$

 ∞

Generalized Lorenz-Mie Theory - GLMT

Expressions of scattered fields

Scattered field

$$E_{\theta} = \frac{iE_0}{kr} \exp(-ikr)S_2 \exp(im\varphi)$$
$$E_{\varphi} = \frac{-E_0}{kr} \exp(-ikr)S_1 \exp(im\varphi)$$
$$H_{\varphi} = \frac{H_0}{E_0}E_{\theta}$$
$$H_{\theta} = -\frac{H_0}{E_0}E_{\varphi}$$

Elements of scattering matrix:

$$-\frac{1}{E_{0}}E_{\varphi}$$

$$\pi_{n}(\cos\theta) \to \pi_{n}^{m}(\cos\theta)$$

$$\tau_{n}(\cos\theta) \to \tau_{n}^{m}(\cos\theta)$$

$$T_{n}(\cos\theta) \to \tau_{n}^{m}(\cos\theta)$$

$$S_{1} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} C_{n} \left[m \left[a_{n}g_{n,TM}^{m} \pi_{n}^{[m]}(\cos\theta) + i \left[b_{n}g_{n,T}^{m} \tau_{n}^{[m]}(\cos\theta) \right] \right]$$

$$S_{2} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} C_{n} \left[a_{n}g_{n,TM}^{m} \tau_{n}^{[m]}(\cos\theta) + i \left[b_{n}g_{n,TE}^{m} \pi_{n}^{[m]}(\cos\theta) \right] \right]$$

Generalized Lorenz-Mie Theory - GLMT

TLM and TLMG for a sphere

Structure of TLMG

Case of a sphere

GLMT for a cylinder

Structure of TLMG

Case of an infinite cylinder

Introduction of the method plane wave expansion

Debye theory

Structure of Debye theory

The Mie coefficients are developed in series, so it is

- a) rigorous,
- b) applied to any wave.

$$\binom{a_n}{b_n} = \frac{1}{2} \left[1 - R_n^{22} - T_n^{12} T_n^{21} \sum_{p=1}^{\infty} \left(R_n^{11} \right)^{p-1} \right] = \frac{1}{2} \left(1 - R_n^{22} - \frac{T_n^{12} T_n^{21}}{1 - R_n^{11}} \right)$$

$$R_{n}^{11} = -\frac{\alpha \xi_{n}^{'}(x)\xi_{n}(y) - \beta \xi_{n}(x)\xi_{n}^{'}(y)}{\alpha \xi_{n}^{'}(x)\zeta_{n}(y) - \beta \xi_{n}(x)\zeta_{n}^{'}(y)} \qquad R_{n}^{22} = -\frac{\alpha \zeta_{n}^{'}(x)\zeta_{n}(y) - \beta \zeta_{n}(x)\zeta_{n}^{'}(y)}{\alpha \xi_{n}^{'}(x)\zeta_{n}(y) - \beta \xi_{n}(x)\zeta_{n}^{'}(y)} T_{n}^{12} = \frac{2i}{\alpha \xi_{n}^{'}(x)\zeta_{n}(y) - \beta \xi_{n}(x)\zeta_{n}^{'}(y)} \qquad T_{n}^{21} = \frac{n_{1}}{n_{2}} \frac{2i}{\alpha \xi_{n}^{'}(x)\zeta_{n}(y) - \beta \xi_{n}(x)\zeta_{n}^{'}(y)}$$

$$b = 0$$
 R_n^{n} T_n^{21} m_1^{n} T_n^{12} T_n^{12} $p = 1$
 R_n^{121} R_n^{121} $p = 1$
 $p = 2$

$$T_n^{21}T_n^{12} = \frac{n_1}{n_2} \frac{-4}{\left[\alpha \xi_n^{\prime}(x)\zeta_n(y) - \beta \xi_n(x)\zeta_n^{\prime}(y)\right]^2}$$
$$\alpha = \begin{cases} n_1/n_2 & \text{pour } a_n \\ 1 & \text{pour } b_n \end{cases} \qquad \beta = \begin{cases} 1 & \text{pour } a_n \\ n_1/n_2 & \text{pour } b_n \end{cases}$$

An **rigorous theory** interprets the scattering in the language of GO.

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ABSphere – software for all physical quantities

Scattering of a pulse by a sphere

Scattering of a Gaussian beam by a sphere

Internal fields

Homogeneous sphere d=40 μm, τ=50 fs Gaussian beam

t = 1080

t = 20

Scattering of a pulse by a sphere

Scattering of a plane wave by a coated sphere

 d_e =40 µm, d_i =20 µm τ =50 fs *Plane wave*

t = -120

t = 20

t = 1060

Scattering of a pulse by a sphere

Scattering of a Gaussian pulse by a sphere

Exercise on geometrical optics

- 1. Under what condition can the geometrical optics be used?
- 2. A light ray arrives on a surface separating two media of different refractive indices. The two figures below represent the reflection coefficients as a function of the incident angle *i* in the two cases: from a more refractive medium to a less refractive and from a less refractive medium to a more refractive.
 - To which case does each of these two figures correspond?
 - What does each of the two curves represent in the figures?
 - Why is there a plateau in the right figure from 41.8°? Deduce the ratio of the refractive indices of the two media.
 - What is the angle of 56.3° in the left figure and 33.7° in the right figure? Explain this phenomenon.
- 3. A light ray of wavelength $\lambda = 0.488 \,\mu\text{m}$ penetrates into a medium of index m = 1.35 0.001i. What is the speed of light in this medium? What is the characteristic depth of penetration defined by $I(\delta) = I(0)/e^{2}$.

