





Monte Carlo Ray Tracing methods for the determination of the radiative properties of materials



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SFT-ACCORT meeting - Paris - Wednesday, November 22, 2017



Laboratoire de Thermique et Energie de Nantes **DU**: Cathy Castelain

8 (+1) C CNRS, 17 EC UN, 4 EC ICAM, 5 IT CNRS- 4 BIATSS UN, 2 IE Cellule CAPACITES LTEN 23 doctorants - 2 ATER/post-doctorants

Transferts thermiques dans les matériaux et aux interfaces (S. Le Corre)

•Transferts aux interfaces et dans les micro-systèmes •Transferts thermiques dans la mise en forme des polymères et composites

 $\mathbb{C} \acute{e} f_0^{p} \mathcal{R}$ am

Metti

ACCOR

Transferts dans les fluides et systèmes énergétiques (L. Luo)

•Transferts chaleur & masse dans les écoulements complexes

•Transferts chaleur & masse dans les fluides complexes Conception et optimisation des systèmes et procédés énergétiques





Professeurs invités





Fév. 2018

Mai 2018

SFT-ACCORT meeting - Paris - Wednesday, November 22, 2017

FédEsol



Contrôle multi-échelle du transport de l'énergie

Caractérisation de la dépendance thermo-spectrodirectionnelle des propriétés radiatives : spectroscopie IR/Vis (réflexion, transmission, émission→ 900 K) D. Hakoume, AO, 2014, J. Mollicone, TSF, 2015 V. Le Louet, IJHMT, 2017

Modélisation multi-échelle des propriétés radiatives : DFT, DM classique, Lorentz-Drude, Monte Carlo, Imagerie 3D

nm → m

B. Rousseau, AIP, 2016, B. Rousseau, AS, 2016 S. Guévelou, IJHMT, 2016, S. Guévelou, JQSRT, 2017 Résolution numérique 3D de

l'Equation du Transfert Radiatif : estimation de propriétés (TO), optimisation énergétique D. Le Hardy, JQSRT, 2016, D. Le Hardy, JCP, 2017 D. Le Hardy, JQSRT, 2017





Some thermal radiative issues...







Δ

How to determine the temperature fields in a part or a component exposed to thermal radiation?



Need to achieve an energy balance between the energy provided by (the) source (s) heating (s) and the illuminated system

> Resolving most often the Radiative Transfer Equation (RTE) in (fluids and solids) semi-transparent media



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Material characteristics



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How can we solve a thermal issue ?





Tseng et al., High Temp.-High Pres., 2013, 42, pp. 387-403

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$$\nabla \dot{q}''(s) = \int_{0}^{\infty} \kappa_{av} 4\pi I_{bv}(T) dv - \int_{0}^{\infty} \int_{4\pi} \kappa_{av} I_{v}(s, \hat{\Omega}) d\Omega dv$$

$$\frac{dI_{\nu}(s,\hat{\Omega})}{ds} = -(\kappa_{a\nu} + \kappa_{d\nu})I_{\nu}(s,\hat{\Omega}) + \kappa_{a\nu}I_{b\nu}(T) + \frac{1}{4\pi}\int_{\Omega'=4\pi}\kappa_{d\nu}P_{\nu}(\hat{\Omega}' \to \hat{\Omega})I_{\nu}(s,\hat{\Omega}')d\Omega'$$





Boundary conditions for RTE solving

$$\begin{split} I \downarrow \nu (s \downarrow p, \Omega) &= e \downarrow \nu I \downarrow b \nu (T(s \downarrow p)) + \int \Omega \uparrow' .n < 0 \uparrow @ \rho \downarrow \nu \uparrow'' (s \downarrow p, \Omega \uparrow', \Omega) \\ I \downarrow \nu (s \downarrow p, \Omega \uparrow') |\Omega \uparrow' .n | d\Omega \uparrow' \end{split}$$



 $\star \rho \downarrow \nu \uparrow S (s \downarrow p, \Omega)$

 $\rho \downarrow \nu \uparrow'' (s \downarrow p, \Omega \uparrow', \Omega) = I \downarrow \nu \uparrow R (s \downarrow p, \Omega) / I \downarrow \nu (s \downarrow p, \Omega) \Omega \uparrow' .n \ d\Omega \uparrow'$

* ρ↓vîD (s↓p ,Ω î')

 $\rho \downarrow \nu \uparrow D (s \downarrow p, \Omega \uparrow') = \int 2\pi \uparrow m \rho \downarrow \nu \uparrow'' (s \downarrow p, \Omega \uparrow', \Omega) \Omega . n d\Omega.$





Kirchhoff law and thermal balance on 1D slab



Heterogeneous material $e \downarrow v (\Omega, T(s \downarrow p)) = 1 - \rho \downarrow v \uparrow D (\Omega, T(s \downarrow p)) - t \downarrow v \uparrow D ($ $\Omega, T(s \downarrow p)$ $\Omega, T(s \downarrow p)) = 1 - \rho \downarrow v \uparrow S (\Omega, T(s \downarrow p)) - t \downarrow v \uparrow S ($ Homogeneous material $e \downarrow v (\Omega, T(s \downarrow p)) = 1 - \rho \downarrow v \uparrow S (\Omega, T(s \downarrow p)) - t \downarrow v \uparrow S ($ $\Omega, T(s \downarrow p)$ $\Omega, T(s \downarrow p)$









Kirchhoff law and thermal balance on 1D slab



Optical thickness $K_{\nu}(T)_{d}$

 $K_{v}(T)d > 1$

Optically thick media opacity

 $K_{\nu}(T)d < 1$

Optically thin media transparency

$$t_{N,\nu}^{S}(T) = \frac{\left[1 - \rho_{a \to m,\nu}(T)\right]^{2}}{1 - \left(\rho_{a \to m,\nu}(T)\right)^{2} \left(\tau_{r,\nu}(T)\right)^{2}} \tau_{r,\nu}(T)$$



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Homogeneous 1D slab, optically polished with parallel faces

$$e_{N,\nu}(T) = \frac{\left[1 - \rho_{a \to m,\nu}(T)\right]\left[1 - \tau_{r,\nu}(T)\right]}{1 - \rho_{a \to m,\nu}(T)\tau_{r,\nu}(T)}$$

$$\rho_{a \to m,\nu}(T) = \frac{(n_{\nu}(T) - 1)^{2} + k_{\nu}(T)^{2}}{(n_{\nu}(T) + 1)^{2} + k_{\nu}(T)^{2}}$$

$$\tau_{r,\nu}(T) = e^{-K_{\nu}(T)d} = e^{-2k_{\nu}(T)\nu d/c}$$

$$\widetilde{n}_{\nu}(T) = n_{\nu}(T) + ik_{\nu}(T)$$



Homogeneous 1D slab, optically polished with parallel faces



Homogeneous 1D slab, optically polished with parallel faces





A model case : silica glass with closed porosity





Geometrical Optics Approximation





Radiative properties computation : MCRT



Monte Carlo Ray Tracing code C++

- Computing time: 10^5 rayons $\rightarrow -40$ s/ wavelength (standard deviation, 0.01)
- Mean free path scattering/absorption
- Scattering phase function
- Scattering geometry

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Absorption/scattering behavior







Agreement between Mie Scattering Theory and MCRT?





Silicon carbide open-cell foams : how can we connect their TRP to their textural features ?



> Chemical composition $\rightarrow \alpha$ -SiC



XRD (PROMES Odeillo, Eric Bèche)





≻2D textural feature





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Textural characterization

(iMorph software : http://www.imorph.fr/)

Porosity= 70%

iusti UMR 7343



Volumetric surface = 2800 m²/m³ • Pore size distribution 0,08 -0.07 0,06 (%) O,05 0,04 0,03 0,02 500 µm 1500 1000 2000 2500 $2r(\mu m)$ • Pore-pore distance distribution 0,05 0,04 PPDD (%) 0.0 0,02 0,01 1000 1500 2000 2500 Mean connectivity of 9,7 $g(\mu m)$ 21 SFT-ACCORT meeting - Paris - Wednesday, November 22, 2017



genMat : a predictive tool for computing emittances from 3D images





genMat : a predictive tool for computing emittances from 3D images





Integral formulation for MCRT?



$$\begin{split} q_{0,\lambda} &= \int_{S_0} dS_0 \int_{2\pi} d\Omega(\vec{\omega}) \ I_{0,\lambda} \ \vec{n}_0 \cdot \vec{\omega} \ \delta(\vec{\omega} - \vec{\omega_0}) = I_{0,\lambda} \\ q_{i,\lambda} &= \int_{S_0} p_{S_0} \, dS_0 \ \left[H(\vec{r}_1 \in S_f) R_1 + H(\vec{r}_1 \in S_i) W_0 \right] \\ R_j &= \int_{2\pi} p_\Omega d\Omega(\vec{\omega}_j) \left[H(\vec{r}_j \in S_f) R_{j+1} + H(\vec{r}_j \in S_i) W_j \right] \\ p_{S_0} &= \frac{1}{S_0} \qquad p_{\Omega_j} = \frac{\delta(\vec{\omega}_j - \vec{\omega}_{j-1})}{\vec{n}_j \cdot \vec{\omega}_j} \qquad W_j = I_{0,\lambda} \ S_0 \prod_{k=1}^j \rho_F(\vec{r}_j, \vec{\omega}_j) \end{split}$$

$$R_{\rm NH} = q_{r,\lambda}/q_{0,\lambda} \qquad T_{\rm NH} = (q_{l,\lambda} + q_{t,\lambda})/q_{0,\lambda}$$

International Journal of Heat and Mass Transfer 93 (2016) 118-129



Representative elementary volumes required to characterize the normal spectral emittance of silicon carbide foams used as volumetric solar absorbers

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iMorphRad : a predictive tool for computing TRP from 3D images

Tancrez et al., IJHMT, 2004, 47, 373–383

RDFI method





How can we go one step further now ?

TRP up to T = 1300 K and not only at T = 300 K !

Numerical foam generator : emissivity→ texture (300 K) ≅ texture (1300 K)

iusti

UMR 7343

Infrared emission spectroscopy (SiC single crystals up to 1300 K)







Numerical foam generator (genMat, C++) \rightarrow p, d_{nom},...

Specific algorithm



grain seed



fast-marching algorithm





segmentation squelettisation Guévelou et al., JPM 2015 ; Guévelou et al., IHTC, Kyoto 2015





Extraction of the dielectric function with an improved Lorentz-Drude model for an heavily doped SiC

MICROSCALE







First oxidation at T = 1700 K, SIC foam p= 70 %





Multi-length scale methods for computing the radiative properties of heterogeneous materials





French Interpore Conference on Porous Media

8 -10 October 2018 - La Cité Nantes Event Center Nantes (France)

Biennial conference

Understanding of the complex behavior of porous media

- > Registration opening and abstract submission : 15th January 2018
- > Deadline for abstract submission : 30th March 2018
- > Notification of acceptance : 13th April 2018
- > Standard registration deadline : 15th June 2018

Ideal place for scientific exchanges where fundamental and applied topics, often interdisciplinary, are discussed :

- > Energy storage
- > Pollution
- Pollution
 Renewable energy
- > Petroleum engineering
 > Natural environment
 > Food and health

> Scientific topics

Mechanical and thermal behavior of porous media - Multi-physics coupling and numerical modelling - Fluid mechanics in Engineering processes - Porous media for energy production and storage - Imaging, numerical generation of porous media - Geotechnical and petroleum engineering - Reactive and dispersive transport - Multiscale fibrous media - Wave propagation



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Cemht

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- S. Le Corre, N. Boyard, D. Delaunay
- D. Hakoume, S. Guévelou, F. Dubot, D. Le Hardy, A. Mekeze-Monthe,
- Md Afeef Badri, V. Le Louet
- J.-Y. Rolland, V. Le Nader, J. Dausseins, A. Biallais







Thank you for your attention ! Some questions?

"Royal de Luxe" Theatre Company : an incredible show at Nantes!



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"Plate" black body





Role of the "macro" roughness : GOA





Role of the "micro" porosity : EMA







RDFI METHOD \rightarrow extinction coefficient, albedo, scattering phase function





Radiative conductivity : optically thick media Rosseland approximation







Future works...

➤To characterize the thermal behavior (conduction/radiation) of SiC open-cell foams above T = 1300 K in relation with degradation mechanisms (corrosion, mechanical failures,...)

➤To play, by numerical modelling, on the surface properties of the struts (roughness, selective/protective coatings) at high temperature

➤To compute thermal conductivities with FEM (Freefem++)

To design foam with pore size gradient : effect on the REV ? \rightarrow 3D printing?



➢Applications with thermal insulators, heat exchangers, radiant gas burners,...



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Materials and Design 44 (2013) 99-106



A simple simulation method for designing fibrous insulation materials

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Five selected papers

2007 : B. Rousseau, D. de Sousa Meneses, P. Echegut, M. Di Michiel, and J.-F. Thovert, "Prediction of the thermal radiative properties of an x-ray μ-tomographied porous silica glass," *Applied Optics*, 46[20] 4266-76 (2007).

2010 : B. Rousseau, H. Gomart, D. Zanghi, D. Bernard, and S. M., "Synchrotron x-ray μ -tomography to model the thermal radiative properties of an opaque ceramic coating at T = 1000 K," *Journal of Materials Research*, 25 1890-97 (2010).

2011 : B. Rousseau, D. De Sousa Meneses, P. Echegut, and J.-F. Thovert, "Textural parameters influencing the radiative properties of a semitransparent porous media," *International Journal of Thermal Sciences*, 50[2] 178-86 (2011).

2015 : S. Guevelou, B. Rousseau, G. Domingues, J. Vicente, G. Flamant, and C. Caliot, "Evolution of the homogeneized volumetric radiative properties of a familliy of α -SiC foams with growing nominal pore diameter "*Journal of Porous Media*, 18[10] (2015).

2017: S. Guévelou, B. Rousseau, G. Domingues, and J. Vicente, "A simple expression for the normal spectral emittance of open-cell foams composed of optically thick and smooth struts," *Journal of Quantitative Spectroscopy and Radiative Transfer*, 189 329-38 (2017)





GDR ACCORT : French research network from CNRS Radiative heat transfer in semi-transparent materials

http://www.gdr-accort.cnrs.fr/





ETR 2017 "Ecole thématique transferts radiatifs en milieux semi-transparents"

Piriac-sur-Mer, France, May 13-19 2017

http://www.etr2017.cnrs.fr/

Responsible : Benoit Rousseau

ETR 2017 Ecole Thématique ETR 2017





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ECOLE TRANSFERTS RADIATIFS EN MILIEUX SEMITRANSPARENTS 13-19 mai 2017 VVF Piriac-sur-Mer

Cette école est organisée dans le cadre du GDR ACtion COncertée en Rayonnement Thermique (ACCORT) qui regroupe dix laboratoires universitaires possédant chacun de fortes activités de recherche, expérimentales et numériques, dans le domaine des transferts radiatifs

Elle vise un public composé d'ingénieurs de l'industrie ou des établissements publics. de chercheurs universitaires et d'étudiants doctorants, confrontés à des problèmes de transferts thermiques où le rayonnement volumique joue un rôle important, notamment dans les matériaux denses ou divisés (mousses, fibreux, céramiques, etc) et dans les gaz, éventuellement en présence de particules (suies, gouttelettes, etc.).

Cette école fera un focus particulier sur la prise en compte des transferts radiatifs dans les matériaux, des nano-échelles aux macro-échelles.









Isotactic PolyPropylene (iPP)* : a multi scale medium for scattering and absorbing thermal radiations





Is there an additional phenomenon than that associated with texture?







Spectroscopie de réflexion/transmission/émission \rightarrow 900 K

