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Comparison of scattering behaviour for spherical and non-spherical particles in pulverized coal combustion

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ABSTRACT

In numerical simulations of coal combustion processes, particle-radiation interaction is often described by Mie-theory. An important modeling assumption in Mie-theory is the sphericity of the particles. The aim of this study is to investigate the validity of the sphericity assumption. Therefore, the T-Matrix method is applied to calculate the scattering and absorption properties of non-spherical particles and to compare these with results from Mie-theory. Three types of non-spherical particles are considered: prolate, oblate, and Chebychev-type particles. The scattering and absorption properties are averaged over a particle size distribution, the incident radiation profile, and for non-spherical particles a particle orientation distribution.

The calculations reveal a deviation in scattering and absorption efficiencies below 10% due to non-sphericity for all particles. For the scattering phase function, the deviation is on the order of 10%. It strongly varies depending on the particle type under investigation. Nevertheless, Mie-theory can correctly predict trends. Taking into account several uncertainties in the input parameters for scattering calculations, Mie-theory can be applied in the prediction of scattering and absorption properties in numerical simulations of coal combustion.

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1. Introduction

In numerical simulations of pulverized coal combustion, the accurate description of radiative heat transfer is crucial to achieve reliable results. This especially applies when particles are considered. Particles vastly increase the complexity by adding scattering to the radiative heat transfer. Mie-theory [1,2] is applied for the description of scattering and absorption efficiencies Q_{abs} and Q_{sca}, as well as for the anisotropic scattering phase function $\Phi(\varphi,\theta)$ by several authors [3–6].

Gupta and co-workers [7] investigated the influence of anisotropic scattering on heat transfer in pulverized coal combustion. The authors applied a Monte Carlo Method to investigate different types of scattering in a furnace with cylindrical geometry, finding that modeling scattering as either forward or isotropic scattering yields large errors, whereas a δ-Eddington type phase function for anisotropic scattering can yield reasonable results. Marakis et al. [8] performed a parametric study for radiative heat transfer in a pulverized coal furnace with a Monte Carlo Method and the P-1 approximation. The authors investigated the influence of different Henyey-Greenstein type scattering phase functions on wall heat fluxes finding that anisotropic scattering should be taken into account in the case of pulverized coal combustion.

The application of Mie-theory includes two important assumptions: sphericity and homogeneity of the particles. Coal consists of organic material (mainly C, N, H, S), minerals and water, distributed inhomogeneously inside the coal (see e. g. Ref. [9]). Ash consists of burnt and partly agglomerated mineral contents of the coal [10], therefore homogeneity is not met. Methods that consider the exact shape and composition of coal and ash particles, as the Discrete Dipole Method (e.g. Ref. [11]), are available but require very high computational effort and detailed knowledge on the composition.

This work has its scope on the investigation of the assumption of sphericity. Scanning electron microscopy studies of burnt and unburnt coal particles revealed that ground coal particles are not

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Nomenclature

Greek symbols

β	Angle determining the rotation of a particle (°)
Δ	Denoting a difference or interval (−)
ε	Sphericity $\varepsilon = a/b$ (−)
λ	Wavelength (μm)
ν	Fluid viscosity (m^2/s)
$\boldsymbol{\omega}$	Particle angular velocity (1/s)
ω	Solid angle (sr)
Φ	Scattering phase function (−)
φ	Polar angle (rad)
ρ	Mass density (kg/m^3)
τ	time scale (s)
θ	Azimuthal angle (rad)

Roman symbols

$\underline{\boldsymbol{A}}$	Rotation matrix (−)
t	length of horizontal axis of a particle (m)
E	distribution of black body radiation, normalized (−)
T	temperature (K)
t	length of vertical (rotational) axis of a particle (m)
C	cross section (m)
D	particle diameter (μm)
s	spread factor in particle size distribution (−)
Δ*D*	local particle interval (μm)
δ	Computational grid spacing (m)
g	gravitational acceleration (m/s^2)
$\underline{\boldsymbol{I}}$	Principal moments of inertial tensor (kgm^2)
$\underline{\boldsymbol{K}}$	Particle resistance tensor (m^3)
k	imaginary part of index of refraction *m* (−)
L	Computational domain length (m)
l	length scale of the flow (m)
m	complex index of refraction (−)
N	number of either wavelength of particle diameter intervals applied. (−)
n	real part of the index of refraction *m* (−)
P(*D*)	particle size distrib. (propability density formulation) (−)
Q	efficiency (−)
R	particle orientation distribution function (−)
Re	Reynolds number (−)
St	Stokes number (−)
$\boldsymbol{T}$	Hydrodynamic torque (kgm^2/s^2)
t	time (s)
$\boldsymbol{u}$	fluid velocity (m/s)
U	mean flow velocity (m/s^2)
$\boldsymbol{v}$	particle velocity (m/s)
x	size parameter $x = \pi D/\lambda$ (−)

Subscripts

η	denoting dissipative length-/timescale
f	fluid
abs	absorption
sca	scattering
Δω	in a solid angle interval
Δφ	in a φ interval
Δθ	in a θ interval
i	index
λ	spectral/wavelength dependent
def	deformed (ε_{def})
max	maximum
Mie	according to Mie theory
min	minimum
m	mean
T	according to T-Matrix Method
V	denoting area of sphere with the same volume
x	x-direction
y	y-direction
P	particle

Superscripts

¯	averaged or integrated Value

Abbreviations

CBK	Char Burnout Kinetics
DNS	Direct numerical simulation
ODF	Particle orientation distribution function

spherical [12]. Ash particles appear nearly spherical but feature bulges or dents, since they often occur as agglomerates of very small particles (D_{ash}=1−3 μm) [10]. According to relevant textbooks [11,13], Mie-theory is valid for description of scattering and absorption of coal clouds in coal combustion simulations. Thereby, non-symmetric behaviour due to non-sphericity of individual particles is assumed to be evened in a cloud of particles. In this work, this assumption is examined by comparison with the T-Matrix code (e. g. Ref. [14]) for non-spherical particles. All particles are assumed to have homogeneous composition.

Irregularly shaped particles and clusters including a size distribution have been investigated before. Hodkinson investigated scattering of irregularly shaped quartz particles suspended in water [15]. An experimental study of polydispersed particles (crystalline silica with a constant real valued refractive index illuminated by visible light) has been carried out and compared to Mie-theory by Holland and Gangne [16]. They found a similarity in scattering coefficients and phase function but poor backscattering predictions for such particles by Mie-theory. Greenberg et al. [17] investigated extinction by rough particles experimentally and compared the results to Mie-theory. Significant differences (up to 40%) in the extinction efficiencies depending on material properties and the size of the particles were determined. Mishchenko et al. investigated the effect of a random orientation of the particles for constant indices of refraction on the scattering and absorption properties as a variable of the size parameter *x* [18]. A cluster of particles was investigated by Mackowski and Mishchenko [19]. Although several investigations on the interaction of non-spherical particles with thermal radiation have been published, the applicability of Mie-theory for non-spherical particles with the refractive index and size of coal and ash has not been reviewed. Additionally, the application of scattering and absorption by non-spherical particles has not been investigated in the context of the finite-volume method for radiative heat transfer thus far.

In the present study, the T-Matrix method is applied to investigate scattering and absorption by coal and ash particles, described as elliptical and Chebychev particles. To achieve results valid for actual numerical simulations of pulverized coal combustion, the conditions in a coal combustion facility are reproduced numerically. Weighting by black body distribution of the incident radiation

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