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Review article

Improving the prediction of environmental fate of engineered nanomaterials by fractal modelling

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ABSTRACT

A critical analysis of the available engineered nanomaterials (ENMs) environmental fate modelling approaches indicates that existing tools do not satisfactorily account for the complexities of nanoscale phenomena. Fractal modelling (FM) can complement existing kinetic fate models by including more accurate interpretations of shape and structure, density and collision efficiency parameters to better describe homo- and heteroaggregation. Pathways to including hierarchical symmetry concepts and a route to establishing a structural classification of nanomaterials based on FM are proposed.

Contents

1. Introduction

Nanotechnology is a field of science and technology involving the design, production and use of structures at the nanoscale (SCENIHR, 2006). Due to the broad applicability of the unique physicochemical characteristics of engineered nanomaterials (ENMs), a variety of nano-enabled applications in electronics, nutrition, cosmetics, medical drugs, food and agriculture, textiles, and energy have been introduced (Hendren et al., 2011; Piccinno et al., 2012). There is concern, however, that the above technological progress may also introduce environmental and human health risks (Klaine et al., 2008). The environmental risk assessment (ERA) used for chemicals is considered as the pertinent approach to assess and quantify environmental risks posed by ENMs (Hristozov et al., 2013; Stone et al., 2014). It is a four-step process, consisting of: 1) hazard identification, 2) effect assessment, 3) exposure assessment, and 4) risk characterization (Van Leeuwen and Vermeire, 2007). Exposure assessment is a fundamental step in the ERA, and

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consists of the calculation of Predicted Environmental Concentrations (PECs). As recommended by the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) Chemical Safety Assessment guidance, dynamic or steady-state multimedia mass balance models (MMMs) are commonly applied to estimate PECs in different compartments. This is due to the fact that in the case of ENMs monitoring information is scarcely available and analytical protocols are still under development (Hassellov et al., 2008; Ono-Ogasawara et al., 2009; Tiede et al., 2010; Tuoriniemi et al., 2012). Physical processes of agglomeration, sedimentation and re-suspension are considered relevant in modelling ENMs environmental fate (Chekli et al., 2015; Meesters et al., 2013; Praetorius et al., 2013, 2012; Quik et al., 2011) but the accuracy of the estimations of these parameters is not satisfactory enough to get realistic predictions (Garner and Keller, 2014).

Meesters et al. (2014) have stressed the relevance of modelling hetero-agglomeration kinetics of ENMs in the water media. A comprehensive analysis of factors affecting ENMs fate, including collision frequency and attachment efficiency is given but the lack of methods capable of predicting structural and surface properties of nanoaggregates is stressed.

To better represent the complexity of nanoaggregate structures in the environment efforts were made to include Fractal Dimension (FD) into the ENMs kinetic models (Arvidsson et al., 2011; Chowdhury et al., 2013; Neil et al., 2016; Praetorius et al., 2012). Nanoparticle (NP) aggregates are less dense material packings in comparison to monocrystals and form structures that are difficult to describe by means of Euclidian geometry. The incorporation of fractal (fractional) dimension demonstrates that the material self-organizes in patterns that cannot fill the granted 3-D space compactly and how much space is truly occupied. However, it does not give insight on the phenomenological processes governing aggregation or on specific morphological properties of particles. Fractal modelling (FM) is often applied to enhance kinetic models (Saunders and Plane, 2006; Sithebe and Nkhalambayausi Chirwa, 2016) but no classification of NMs based on fractal properties has yet been proposed.

The goals of this paper is to identify how limitations of existing approaches used for the predictions of ENMs fate may be overcome with the help of FM. Specifically, this paper will (i) present the existing methods employed for ENMs exposure and fate modelling, (ii) introduce basic concepts and methods of fractal geometry and (iii) describe the pathways of applying FM to obtain more realistic predictions of ENMs environmental behaviour.

2. Towards the incorporation of fractal modelling in transformation and transport kinetics models

2.1. Existing modelling approaches in ENMs environmental fate and transport

Modeling methodologies applied so far to ERA consider mainly Mass Flow Analysis (MFA). Mueller and Nowack (2008) developed the first material flow model considering releases of ENMs from products in different lifecycle stages to estimate PECs for nanoscale Ag, TiO_2 and Carbon Nanotubes (CNTs) in the Swiss air, soils and waters. Later this approach was applied to budgeting environmental distribution of ENMs in Denmark (Gottschalk et al., 2015). Further developments overcame the simple approach by addressing input uncertainties for a holistic spectrum of possible scenarios through a probabilistic model involving Monte Carlo, Bayesian and Markov Chain analyses (Gottschalk et al., 2009, 2010). In Keller and Lazareva (2014) this modelling approach is applied to predict region-specific environmental concentrations. The models incorporate input parameters such as production and consumption volumes, fate pathways quantified though transfer coefficients. However, it is stressed that relevant factors of engineered nanoparticles' (ENP) size, structure, chemical activity and evolution in the environment are not taken into consideration. To model such parameters, new mechanistic approaches (Maggi, 2009; Sithebe and Nkhalambayausi Chirwa, 2016) that would take specific physical and chemical nanoscale phenomena (Bishop et al., 2009; Walker et al., 2010a) into consideration are needed.

Kinetic models were applied in Quik et al. (2011) to introduce dissolution and sedimentation rate constants seeking a step-by-step environmental fate simulation. This approach represented a move toward defining exposure in the aquatic environment but did not provide the possibility to describe the transport of ENMs and accordingly predict their behaviour in different media. Arvidsson et al. (2011) proposed the use of kinetic laws by Smoluchowski (1917) and Friedlander (2000) along with the inclusion of sedimentation, perikinetic and ortokinetic agglomeration caused by shear flows and differential settling caused by sedimentation into account.

In later work, Praetorius et al. (2012) added ENM interactions with suspended particulate matter (SPM) to the model. Definitions for rate constants were derived from Elimelech et al. (1995a). Aggregation with environmental colloids is more frequent than interaction between the pristine particles, and the lack of a systematized approach to describing physical aspects of the phenomena responsible for these interactions makes accurate fate predictions a complicated task (Docter et al., 2015, Jun et al., 2016).

2.2. FM applied to aggregation modelling

The first steps to account for the shortcomings related to shape and topology were made by including fractal dimension into the kinetic equations as a statistical parameter (Arvidsson et al., 2011; Praetorius et al., 2012). Wiesner (1992) and Elimelech (1995a) were among the first to introduce FD-dependent floc density when modelling nano- and micro-scale aggregation. According to Wiesner (1992), the mass density ρ of a sphere of radius r within a floc is a power function

$$\rho(r) \sim r^{(D_f - 3)}$$

where fractal dimension D_f can take values from 1 to 3. This shows that the material occupies less volume within the Euclidian space than an entirely compact object such as a coalesced sphere. The value of fractal dimension is obtained with the same equation that gives the dimension of objects in the Euclidian space. When an object is split into N equal parts that are r times smaller than the original object the dimension D of the object is defined as:

$$D = \frac{logN}{log(1/r)}$$

$D = 2$ for a compact plane, and 3 for a compact cube. In the case of less dense objects for a large enough r dimension would take fractional values, accounting for the space not occupied by material, and would be called fractal dimension (FD) (Crownover, 1995). It is also used as a measure of complexity for structured non-compact mathematical objects, especially those completely or partially self-similar at any scale of examination, called fractals (Mandelbrot, 1983). FM uses various iterative algorithms to build such complex structures.

The first methods applied to physical aggregation modelling were based on the concepts of the Diffusion Limited Aggregation (DLA), proposed by Witten and Sander (Witten and Sander, 1981; Frenklach et al., 2009; Köylü et al., 1995; Pippa et al., 2013) where particles moving in Brownian motion stick together in case of collisions (Fig. 1). The process is chaotic, however by modifying the rules of attachment and disattachment the FD dimension can vary (Inci et al., 2014).

Deterministic fractals with a strictly defined symmetry are an alternative to DLA. The idea of using self-similarity and self-affinity to model nanosystems has been presented by Mandelbrot (1986). In the mentioned work an object is defined as self-affine if it consists of non-overlapping parts that can be represented by applying a linear affine

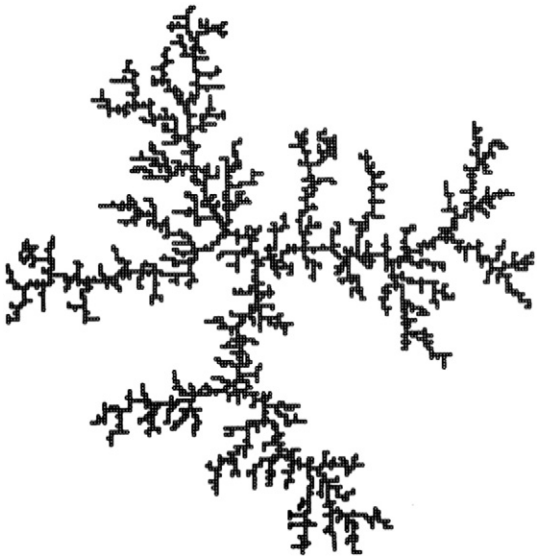

Fig. 1. A DLA model of a 3000 particle aggregate on a square lattice. Courtesy of Witten and Sander, 1981.

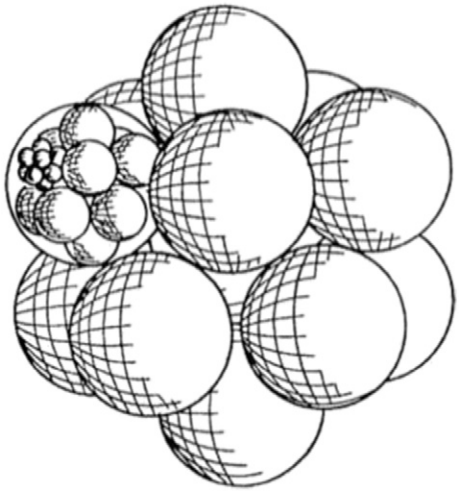

Fig. 2. A conceptual representation of a self-similar and self-affine hierarchical object. Courtesy of Shevchenko and Mackay (2011).

transformation function (combination of translation, scaling and rotation operations) to other parts of this object (Fig. 2).

As shown in methodological works of Barnsley on the Iterated Functions System (IFS) method (Barnsley, 1988; Barnsley and Demko, 1985; Nikiel, 2007) the recursive process of applying such transformations from a predefined set to a primary particle builds traces of fractal objects with a desired symmetry (Fig. 3a).

Fractals (Fig. 1, 3a) are inherently characterized by a fractal dimension. The common method to calculate FD of fractal models is the Box-Counting method when the studied object is repeatedly covered with sets of boxes, and each set is defined by the size of the box's edge, r. The number of boxes N necessary to cover the object is plotted as a function of r and the slope S of the $\log(N(r))/\log(r))$ graph gives the FD, in this case called box fractal dimension (Jelinek et al., 2013; Feder, 1988).

The relevance of fractals for the nanoscale is linked to the morphology-specific physico-chemical properties that distinguish them from chemicals and before a NP dissolves (Dale et al., 2013) colloidal aggregation should be accounted for (Cai et al., 2017; Wang et al., 2003). By now fractal dimension is included in various NM studies, e.g. evolution studies of nanoscale TiO_2 in aquatic media (Chowdhury et al., 2013; Godinez and Darnault, 2011; Loosli et al., 2013; Xu et al., 2014), studies of fullerite nanoparticles in electrolyte solutions (Meng et al., 2013). Fractal image analysis methods were used to classify organic and inorganic structures (Kimori et al., 2011; Kong et al., 2014; Papanicolaou et al., 2012; Smith et al., 1996, Neil and Curtis, 1997). Neil et al. (2016) studied fractal structures of iron oxide nanoparticles aggregated with natural organic matter and arsenate to better predict the sedimentation rates in the environment. The oil industry recently adopted fractals to enhance environmental kinetics models (Mohammadi et al., 2016; Sterling et al., 2005). Fractal parameters are used to realistically mimic nanosystems in biology, medicine and pharmaceutical sciences (Graham and van Ooyen, 2001; Jayasuriya et al., 2013; Pippa et al., 2013; Captur et al., 2015; Kaandorp, 1994; Karperien et al., 2013).

2.3. Introduction of a fractal classification of ENPs aggregate structures

The last mentioned work of Karperien et al. (2013) is focused on developing a classification of neuron cells based on their fractal shape. This approach is feasible as such representations of cells require little amounts of hard-drive storage (fractals are represented by functions that can be written in a text file) and give a comprehensive description of the cell's structure.

To develop such a classification for ENMs, a structure analyzing method should be applied. One of the first applications of fractals was image compression, and many specialized image processing methods

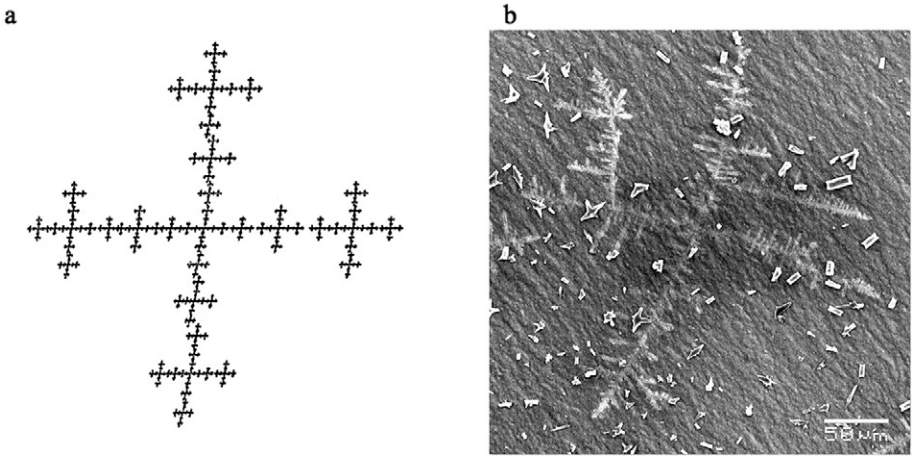

Fig. 3. (a) A 2D IFS model of a dendrite cluster. (b) A SEM image of the modelled $CaSO_4$ – H_2O – CNT hybrid material with the corresponding symmetry. Courtesy of Bitutskaya et al. (2013).

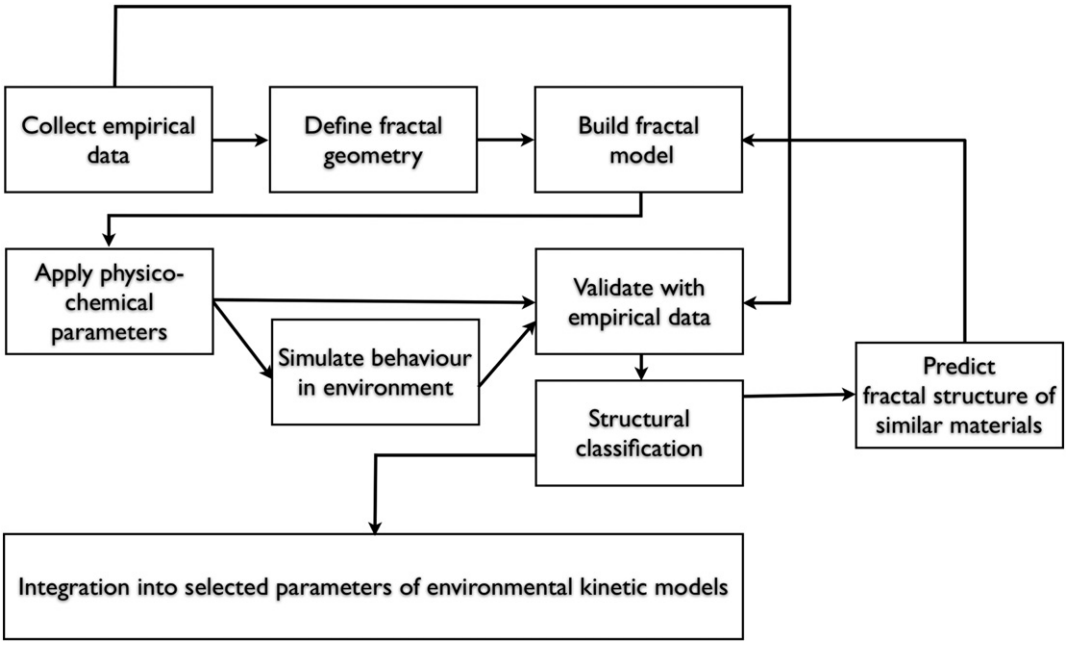

Fig. 4. A schematic of the proposed route for the integration of fractal modelling into environmental kinetic models.

were developed (Ho Moon et al., 1999; Papanicolaou et al., 2012; Smith et al., 1989; Xiaoqing et al., 2013). A good example of a well applied fractal classification are fingerprint databases (Lin, Chen and Gaing, 2010). The process of building a fractal model is rapid as it is based on recursive algorithms. For instance, an array of 50000 pixels requires less than 8 seconds to be built using the IFS method and rendering algorithms for various FM methods are constantly optimized for productivity (Gröller, 1994; Karam and Nakajima, 2001; Martyn, 2010).

These considerations predict a possibility to develop and apply a quantitative structure classification of nanomaterials to include in kinetic transport and transformation models used in environmental fate modelling. A schematic representation of the predicted steps is given in Fig. 4. Further Table 1 focuses on how various parameters used in existing environmental models (Dale et al., 2015) could benefit from FM and nearest steps required for an integration are presented in more detail in Section 3.

3. Steps to include FM in ENM environmental kinetic models

In this section nearest steps required to fulfill the tasks resulting from the schematic approach shown in Fig. 4 are presented.

3.1. Step 1. Collecting empirical data and building the fractal model

The lack of quantification methods for creating a nanoaggregate morphology classification was stressed by Pippa et al. (2013) and Papanicolaou et al. (2012). Currently technology provides powerful methods to study material structures. For example, Fig. 5a shows a Cryo-TEM tomography reconstruction of an organic nanoparticle. This 3-D image can be analyzed to find a characteristic symmetric algorithm.

The Polar IFS and the Generic Programming image-decoding methods are capable of solving the task of defining an IFS for a given image (Collet et al., 2000; Hart, 1996; Hart et al., 1997). An electron microscopy image of an aggregate can also be reduced to its outlines to simplify the analysis (Kimori et al., 2011; Du et al., 2012; Ferreiro et al., 2013; Hagerhall et al., 2004). The symmetry types can be extracted from new geometrical theories developed for new tasks in material engineering (Lord et al., 2006; Shevchenko and Mackay, 2011; Ivanov and Talanov, 2013; Bokeloh et al., 2010).

In the given example (Fig. 5a), the symmetry is icosahedral and a fractal model with a corresponding symmetry can be created. In the self-affine approximation the model (Fig. 5b) represents the real particle's structuring.

It was shown that NMs do not maintain ideal symmetrical structures, and form semi-chaotic structures (Mandelbrot, 1992; Walker et al., 2011). However, taking into account the appearance frequency of polyhedral objects in the nanoscale world (Kowalczyk et al., 2011; Walker et al., 2010a, 2010b) the deterministic FM approaches (Karperien et al., 2013; Avilov et al., 2014) can be considered applicable for aggregation modelling. The IFS fractal generation process is based on a chaotic algorithm that allows for variability and provides realistic uniqueness to every modelled object while sustaining a general symmetrical pattern.

The turtle graphics (L-system) method that builds branching systems according to a pre-defined rule (Ju et al., 2004; Crownover, 1995) could be an alternative to the IFS models. It was found applicable in the modelling of neuron structures (Karperien et al., 2013).

3.2. Step 2. Linking physico-chemical characteristics to the fractal model

Environmental fate and exposure modelling of ENMs deals with an abundance of variables and the aim is to find simple enough approaches that would streamline this complexity (Sani-Kast et al., 2015). However even given the possibility to model complex fractal structures it is necessary to functionalize them with relevant physical and chemical properties.

The DLVO theory is used in MMMs to addresses the colloidal stability through the description of the interactions experienced by a nanoparticle when approaching another nanoparticle or a collector surface. The classical DLVO theory (Petosa et al., 2010) takes only van der Waals and electrostatic interactions into account, whereas the revised version of the theory additionally considers other specific interactions that are relevant when dealing with NMs, such as magnetic forces, steric

Table 1
The table reports definitions of the descriptors used in MMMs and improvements that can be introduced to these descriptors by FM.

Descriptors relevant for ENMs fate modelling	Approaches from MMMs	Predicted FM improvements
Particle shape	Particles are assumed to be spherical (Arvidsson et al., 2011; Liu and Cohen, 2014; Praetorius et al., 2012).	Aggregates are to be represented as complex self-similar hierarchical deterministic symmetric or chaotic objects (Gmachowski, 2002; Mandelbrot, 1992).
Density	Density is given as a constant. Fractal dimension is introduced as a coefficient to better represent how aggregates occupy the given volume (Arvidsson et al., 2011).	Floc density can be predicted from the morphology and FD of the fractal models. Pores and voids that influence material density are often hard to study experimentally whereas they can mathematically predicted with the use of fractal models (Pia et al., 2016).
Particle size distribution	Describes how the size of the individual particles varies in a dispersion (Linsinger et al., 2012).	Deterministic fractals predict stable characteristic sizes (Li et al., 2016) within modelled structures basing on the chosen symmetry and hierarchical scaling properties.
Initial particle shape and size	Also mentioned as primary particle size (Praetorius et al., 2012) or crystallite size (Linsinger et al., 2012), it corresponds to the diameter of the primary particles of which aggregates are formed.	Dots in fractal models can be replaced with monocrystal or amorphous particles of the initial size and shape and corresponding physico-chemical parameters can be linked (ISO, 2012; Mishin et al., 2015).
Break-up and limiting size	It is defined in (Elimelech et al., 1995b) as the maximum size of aggregates that depends on the applied shear or energy dissipation and on “floc strength”, also dependent on the attractive forces between particles.	Particle break-up can be predicted if forces responsible for aggregation and disaggregation (Li et al., 2016; Bishop et al., 2009; Walker et al., 2011) are applied and binding forces between the models and model parts are evaluated for both homo- and heteroagglomerates.
Collision frequency	It is a second-order rate constant, which depends on a number of factors, such as particle size and transport mechanisms. Recent studies of particle functionalization in the environment (Docter et al., 2015; Nasser and Lynch, 2016) stress the need to model physicochemical properties in order to predict the real size of functionalized particles in the environment.	In (Elimelech et al., 1995b) it is shown that the real volume occupied by aggregates tends to be higher than that of the smaller particles summed together, thus a more realistic prediction of an overall collision frequency can be achieved if fractal dimension and structuring are taken into account when calculating particle volume.
Collision efficiency also referred to as "sticking probability" or "stickiness coefficient", α	It is defined as the fraction of collisions that are effective in agglomeration in (Elimelech et al., 1995b). Praetorius et al. (2012) and by Quik et al. (2011) refer to it as attachment efficiency.	Predictions of collision efficiency can be made if physico-chemical characteristics (Buffle et al., 1998; Stolpe and Hassellöv, 2007) are applied to the modelled particle's surface area and binding forces with other particles are calculated. The descriptor is used in DLA models (Witten and Sander, 1981) as an input parameter.
Composition	The chemical nature of the materials. Recent studies show that the composition of the eco-corona (Docter et al., 2014; Nasser and Lynch, 2016) is highly relevant for ENMs fate in the environment. The protein corona may be considered the endpoint of ENPs within a live organism (Canesi and Corsi, 2016), thus it is relevant for risk assessment.	The surface chemistry properties of modelled nanoparticles are defined by the properties of the comprising material (Lin, Tian, et al., 2010; Tuchin et al., 2014). Also the parameter of composition can be used to predict self-assembly patterns (Walker et al., 2010b) if a classification of NMs is produced, and vice versa.
Homo- and Hetero-agglomeration/aggregation rate constants	Mentioned in (Arvidsson et al., 2011) as the rate constants governing agglomeration/aggregation processes. Homo-agglomeration/aggregation refers to interactions of ENMs of the same type; hetero-agglomeration/aggregation is the interaction of ENMs with natural colloids and SPM.	A structural classification of ENMs and relevant environmental particles with linked physico-chemical parameters can help develop an algorithm to predict the stability of aggregation between nanomaterials and particles of similar and different composition (López-López et al., 2006; Zhang, 2014; Smith et al., 2015).

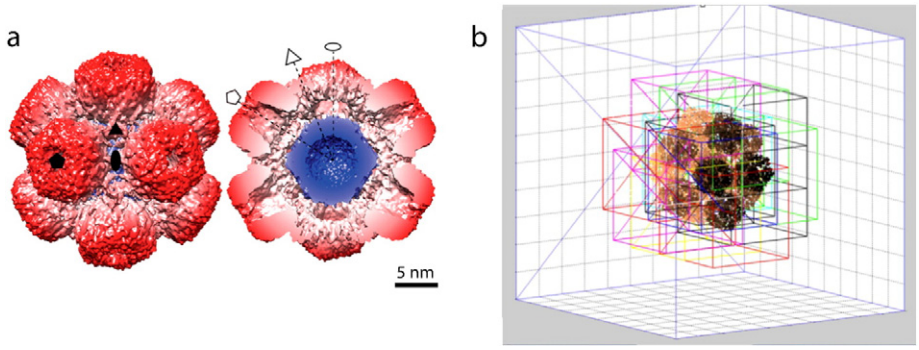

Fig. 5. a) A Cryo-TEM tomography reconstruction of a protein-RNA nanoparticle with an icosahedral symmetry. Pentagon, triangle and oval symbols indicate the icosahedral symmetry axes. Courtesy of Kler et al. (2013). b) An IFS fractal dot model with an icosahedral symmetry. Array of 80000 pixels. Colored overlapping cubes depict the transformations that the 13 affine functions would apply to a larger primary unitary cube. Courtesy of Avilov et al. (2014).

interactions, and hydration forces (Grasso et al., 2002, Bishop et al., 2009; Healy and White, 1978; Lin and Wiesner, 2012).

Apart from the listed forces, there are other nanoscale-specific phenomena that are to be taken into consideration. For example, in (Browne and Grzybowski, 2011; Walker et al., 2013; Wang et al., 2011) it is shown how curvature of nanoparticles impacts electrical field distributions and the character of aggregation for various materials. Modelling by Tuchin et al. (2014) and Zhukalin et al. (2014) for carbon nanotubes shows that curvature at the nanoscale governs the redistributions of surface electric fields. Length- and diameter-dependent oscillations of the band gap and the subsequent altering of chemical properties for nanotubes were described in Ganin et al. (2014). More accurate shape considerations would improve predictions of chemical reactivity that can depend on surface energy for nanocrystals (Pal et al., 2007; Solla-Gullón et al., 2008; Xu et al., 2006).

The importance of the primary cluster morphology for aggregate evolution was shown in (Brasil et al., 2001) where a characteristic attachment angle parameter was defined for carbon soot particles. In the self-affine approximation, the relative arrangement of the affine reflections that form the fractal model can be chosen to correspond with the attachment angle. The initial monocrystals are then considered information carriers, responsible for the subsequent symmetrical aggregate self-assembly (Walker et al., 2010b, 2010a).

This approach to modelling hierarchical nanoparticles enhanced by physicochemical functionalization can be further applied to modelling heteroaggregation (Bitutskaya et al., 2013; Patil and Mann, 2008; Ruiz-Hitzky et al., 2008). Experimental evidence (Bitutskaya et al., 2013; Neil et al., 2016) shows that during the formation of hybrid nanosystems NMs can rebuild their structure depending on the intrinsic qualities (i.e. shape, dispersability) of the components. From the modelling point of view, it could be described as an integration of two (or several) characteristic symmetries and the formation of a qualitatively and quantitatively new symmetry. More specific experimental data is needed to develop and validate this approach to modelling hetero-aggregation. As shown in Bitutskaya et al. (2013) and Zhukalin et al. (2014) symmetry modifications can depend on component concentrations, pressure and other parameters.

3.3. Step 3. Validation and application

A created model should be verified with experimental data before incorporating it into a structural database and making predictions of structures of similar composition or properties.

In environmental kinetic models (Arvidsson et al., 2011; Praetorius et al., 2012) the volume and, subsequently, density of fractal aggregates are linked to FD, that itself is dependent on aggregate morphology. Then the same methods used to measure floc volume and density should be applied *in silica* for fractal models. Given the chemical composition of the modelled material and the initial particle shapes and sizes, a mass value can be calculated for the volume occupied by the modelled fractal morphology. The measured and calculated densities are then compared to validate the model. Important to note that density is a complex parameter as it depends on the experimental conditions and material packing. In nanosystems density is often quantified in molecules/nm^3, not in g/ml and can change depending on coatings (Park et al., 2004; Zhuravlev and Potapov, 2006).

The same algorithm can be applied to compare measured and modelled electro-physical parameters of surface charge, zeta-potential, etc.

In Kowalczyk et al. (2009) and Bishop et al. (2009) it was stated that the sizes of NPs likely to aggregate tend to stay within one scaling level, i.e. after reaching a certain limit larger particles loose reactivity with smaller particles, but they may be able to agglomerate with one another. A relation between scale and binding force was shown in Kalsin et al. (2006) where ordered non-compact structures were observed for larger aggregate sizes of silver and gold NPs. This demonstrates the scale selectivity of physico-chemical interactions at the nanoscale and could be another validation algorithm, in which characteristic stable aggregate sizes are compared with characteristic sizes of the hierarchical fractal models.

The values of the physico-chemical constants obtained from fractal models can then be used when solving environmental kinetics equations as input parameters and factors affecting statistical descriptors mentioned in Table 1 to achieve more accurate ENM fate predictions.

4. Conclusions

The critical analysis of the available ENMs environmental fate modelling approaches presented in this work confirms that existing tools do not satisfactorily reflect the complexity of relevant nanoscale aggregation phenomena. It has been shown that FM would provide a more realistic representation of NP aggregate structures, and steps to apply a fractal-based NM classification to improve existing kinetic models were proposed. A listing of descriptors from existing MMMs that can be described more accurately with FM was given. The presented approach in modelling is applicable to non-compact colloid aggregates, however fractal image analysis may be more broadly used for the detection of specific ENMs in the environment.

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