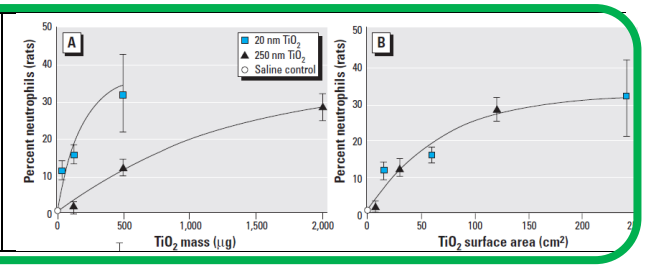
Particle Surface to characterize Biologic Activity of Aerosols, in particular of Combustion Soot - but which Surface ?

Andreas C.R. Mayer
Dipl.Ing, SAE-fellow, Dr.med.hc

G.Oberdörster (Env.Health 7/2005) demonstrated that nanotoxicology is linked to particle surface, not to mass PM. But which surface? He links it to BET surface, the multimolecular nitrogen absorption surface (Brunauer, Emmet, Teller, J.of Am. Chem.Soc. 2/1938), including all hidden surfaces like open porosity. Maybe he would agree to "protein accessible surface" but surely not to geometric surface or Fuchs-surface or LDSA = lung deposited surface area. .

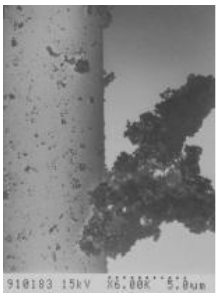


Spherical Particles, formed e.g. by condensation generate well-defined monodisperse or polydisperse aerosols. Size, number, shape, surface, density are perfectly described. The specific surface increases with size-reduction and may reach 300 m^2/g with 20 nm at a density of 1 g/cm^3 (activated charcoals with open porosity reach 3000 m^2/g) **This implies: "size matters" - smaller particles have higher biologic impact probability.**

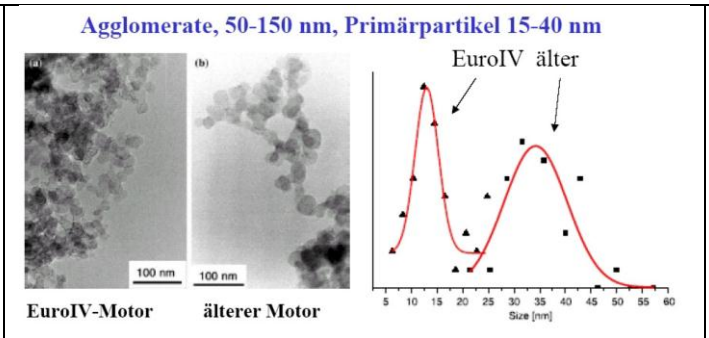
Total Mass (g / cm³)	Particle Size (µm resp. nm)		Number of Particles per cm³	Total Surface (µm)²
8 x 10^{-12}	2.5 µm	2500 nm	1	20
8 x 10^{-12}	0.5 µm	500 nm	125	100
8 x 10^{-12}	0.1 µm	100 nm	15'600	500
8 x 10^{-12}	0.02 µm	20 nm	1'953'000	2'500

G.Leutert

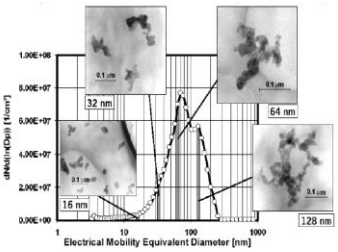
But Soot is different: *BET is constant, independent on particle (agglomerate) size*



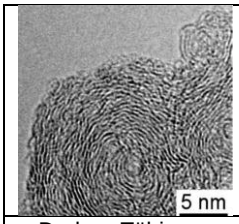
Soot Agglomerate on a filter fiber J.Mayer



MAN: soot of two Diesel engine generations: similar agglomerates with slightly different primary particle diameter 20 ± 10 nm



N.Metz: larger particle size means more primary particles nothing else



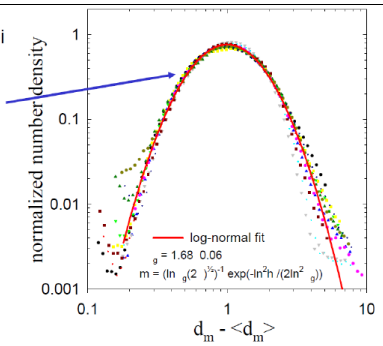
Dreher, Tübingen

Beauty of Fullerenes

The primary particle itself, generated within microseconds in the oxygen-poor zones by graphite like hexagonal/pentagonal layers, starting with PAH structures but later dehydrated, is forming spheres morphologically similar to onion shells (Siegmann, ETH). This structure is dense, providing no internal open pore surfaces, has a density of 2 - 2.5 g/cm^3 (Pauli, Diss. Aachen) and BET surface is "only" 200 m^2/g and in contrast to many other aerosols the active surface BAT can be easily calculated.

Probably a not very active surface – unless coated by PAH and metal clusters

- PMP method removes nuclei particles
- Remaining solid particles follow lognormal distribution with 2 free parameters
  - Number
  - Mean diameter
- Mean diameter between ~40 – 80 nm
- To fulfill number standard of $5x10^{11}$ #/km → PM mass must be < 1 mg/km



Mass = N π/6 ρ_0 $d_0^{(3-df)}$ μ_g^{df} exp(df^2 $(\ln\sigma_g)^2/2$)

M.Maricq (Aerosol science 4/2004 and HEI 5/2009) summarizes the knowledge on soot, assuming the widely proven lognormal size distribution of engine emitted soot and comes up with a formula to calculate mass from number with some assumptions on agglomerate shape (df) He claims that this calculation is more accurate to conclude on PM than gravimetric PM direct measurement.
This means:
once we know the particle mass measured or calculated from PN (following Maricq) and since we know the specific BET of soot (which is constant within little variance) we can conclude on total BET of any soot aerosol in m^2/m^3 per aerosol volume flow which is the correct value for biologic impact other than Fuchs or LDSA

BET specific surface m^2/g of soot is independent on particle (agglomerate) size - constant ≈ 200 m^2/g
BET surface of a combustion soot aerosol sample m^2/m^3 can be calculated based on PN only
But geometric surface is not enough to define specific surface reactivity (Oberdörster, NanoImpact, 10/2018), since there might be strong physical, chemical or biological activation to multiply the surface effects, concluding size is responsible for translocation, activated surface for health impact – representing **the Trojan Horse Effect**

Andreas Mayer / VERT - Ttm.a.mayer@bluewin.ch - +41 56 4966464