Application of a Quantum Statistical Model of Humic Substances to their Influence on Reduction of Red Cell Aggregation in Blood

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1. Aim and scope
2. Data
3. Quantum statistical modeling of HS
4. Application of proposed concept
5. Conclusions

1. Aim and scope

Among various remediation factors, humic substances has substantial effect on the environmental contamination significantly changing the contaminant's degradation, bioavailability, reactivity, and mobilization.

Their remediation effect in water solution (surface waters) strongly depends on:

- HS concentration in water;
- Aromaticity index of HS.

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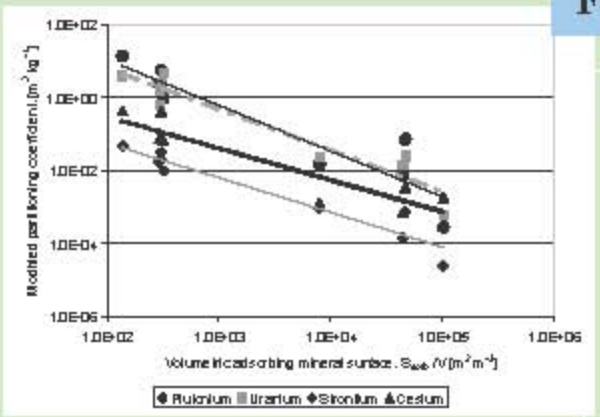
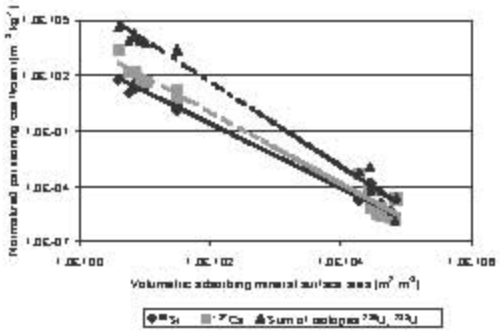
Objective: understanding of physical, chemical and biomolecular processes that define influence of HS concentration on their remediation effect.

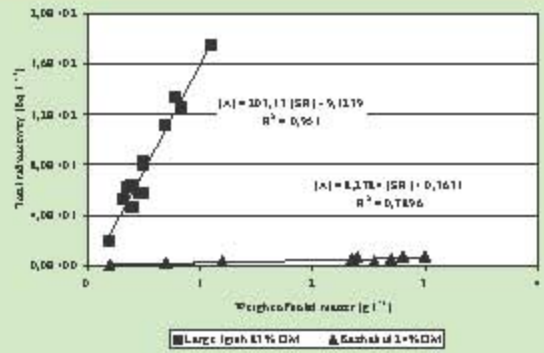
2. Data

For lakes and surface water reservoirs of South Ural, Russia



Regression of the modified partitioning coefficient $K_d/(m_{HS}/m_{HS(0)})$ on the volumetric adsorbing surface area





Scatter plot of total radioactivity per volume in dependence on weight of solid phase in lake Large Igish (83% of SR is OM) and Kazhakul (24% of SR is OM)

$$K_{d\_RN} \cdot \frac{m_{HS(0)} / s_{(0)}^{1-\alpha_{RN}}}{m_{HS} / s^{1-\alpha_{RN}}} = const$$

$$A_{RN\_sorb} = const \cdot \frac{m_{HS} / s^{1-\alpha_{RN}}}{m_{HS(0)} / s_{(0)}^{1-\alpha_{RN}}} \cdot A_{RN\_diss}$$

➢ **An increase in the local HS concentration results in an increasing of the local volumetric activity of RN bound to solids…**

O.N. Aleksandrova, M.Schulz, M. Matthies. Journal of water air soil pollution (2010) 206: 203-214; (2008) 194; 287-299

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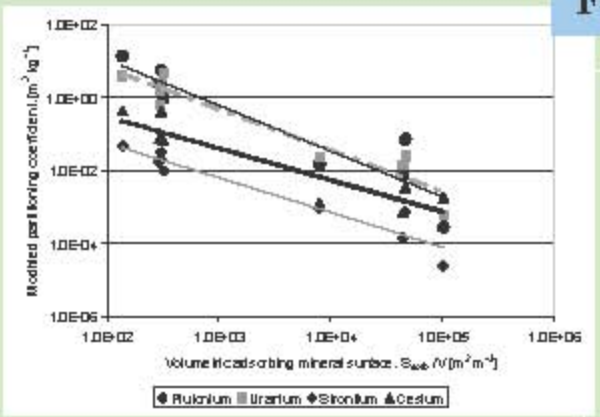

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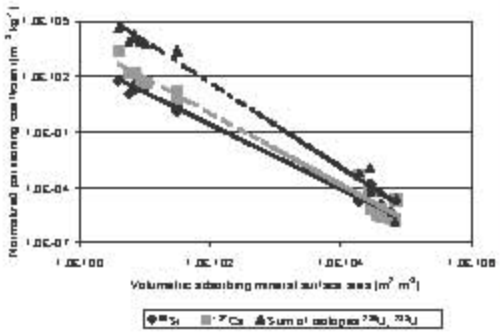

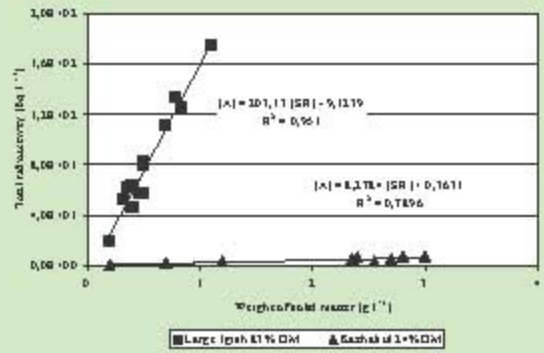

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- **However…**

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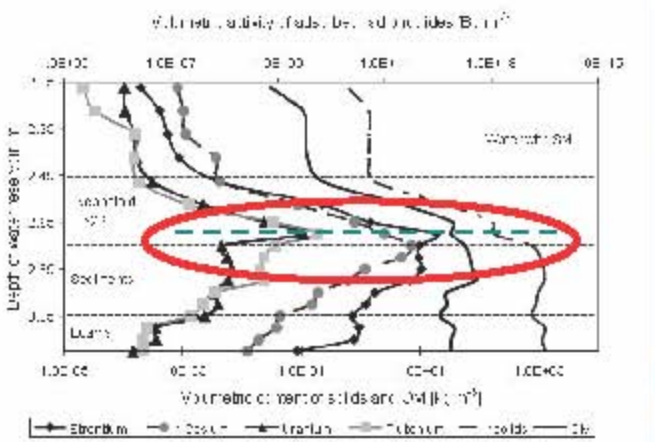
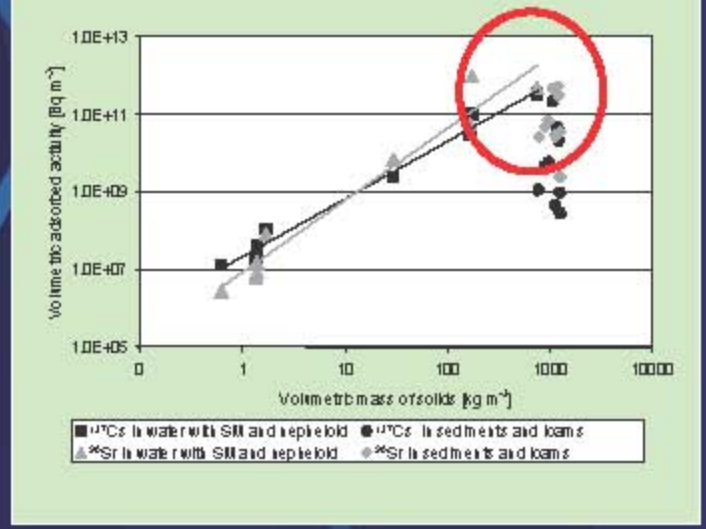


Depth profiles of the volumetric activity of RN bound to solids and the volumetric content of solids and organic matter (OM)



Regression of the volumetric adsorbed activities of radionuclides 90Sr and 137Cs on the volumetric content of solids (SR)

- **An increase in the local HS concentration results in an increasing of the local volumetric activity of RN bound to solids.**
- **However, when the HS concentration exceeds the definite value solid phase containing HS begins to lose some radionuclides.**

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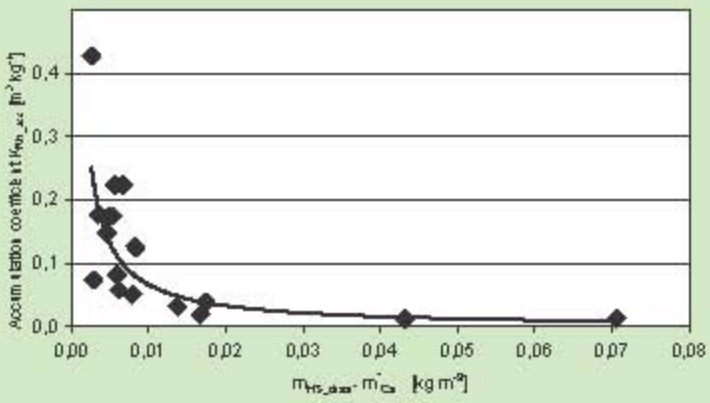

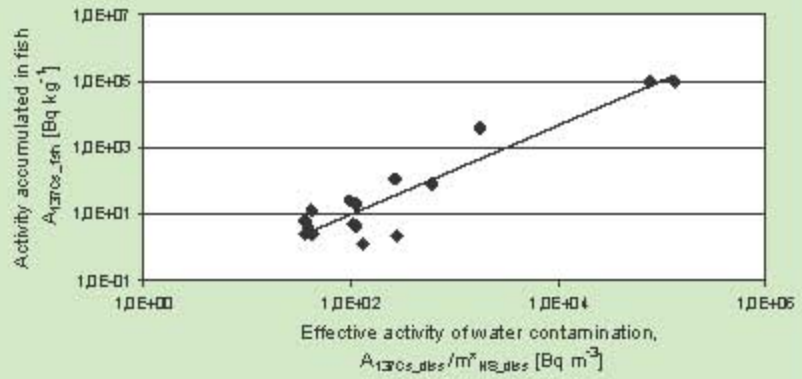

$$[K_{RN\_acc}] = 0.0007 \cdot [m_{HS\_diss} \cdot m^{*}_{Ca}]^{-0.9819}$$

R^2=0.7241

$$[A_{^{137}Cs\_fish}] = 0.0204 [A_{^{137}Cs\_diss} / m^{*}_{HS\_diss}]^{1.3411}$$

R^2=0.8744

➢ **An increase in the HS concentration results in decreasing of bioaccumulation of RN in fish as**

$$K_{RN\_acc} = A_{RN\_fish} / A_{RN\_water} \sim 1/m^{\beta}_{HS\_diss}, \beta \geq 1$$

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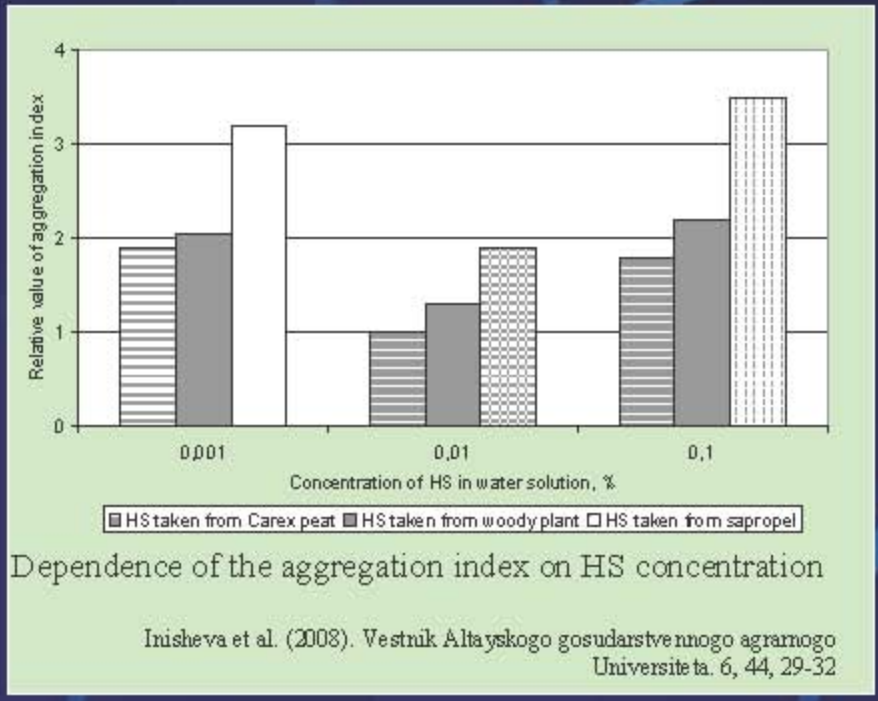
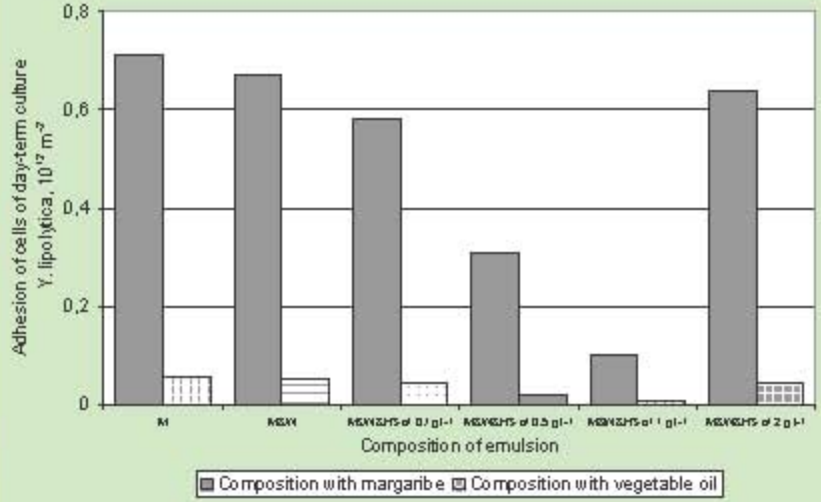


Dependence of the aggregation index on HS concentration

Inisheva et al. (2008). Vestnik Altayskogo gosudarstvennogo agrarnogo Universiteta. 6, 44, 29-32



An effect of different HS concentrations on the adhesion of cells (~ 10^7 colony assay pro ml) by emulsion drops

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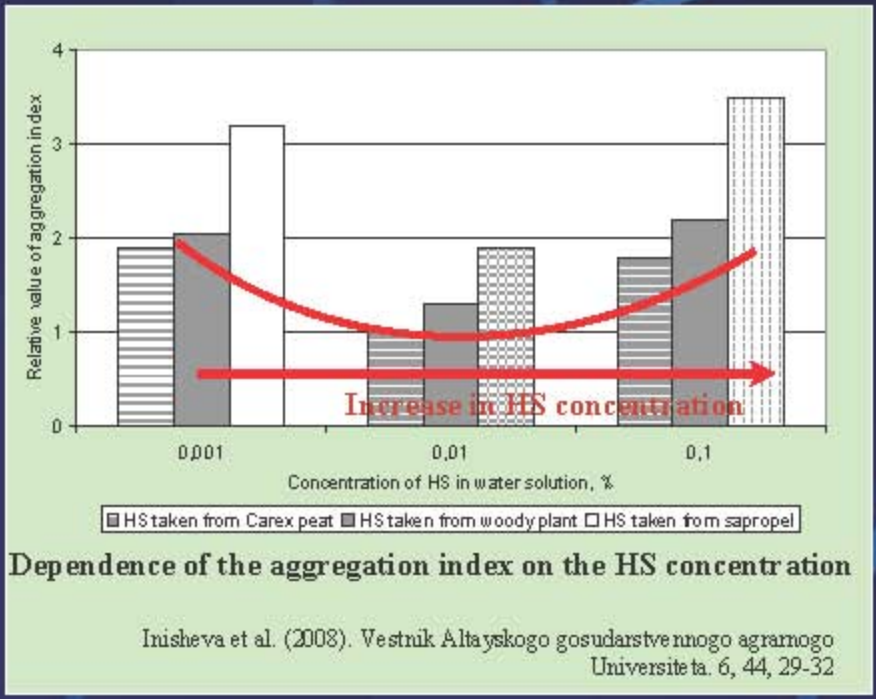

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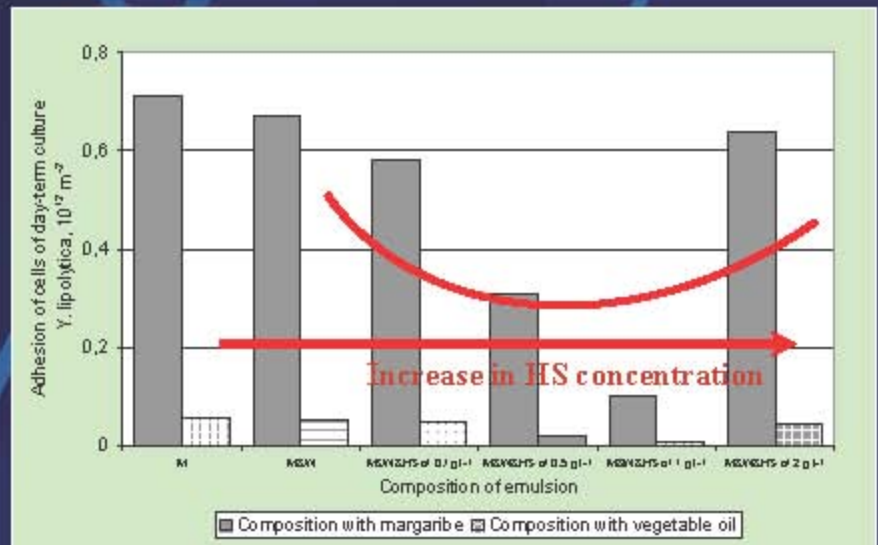

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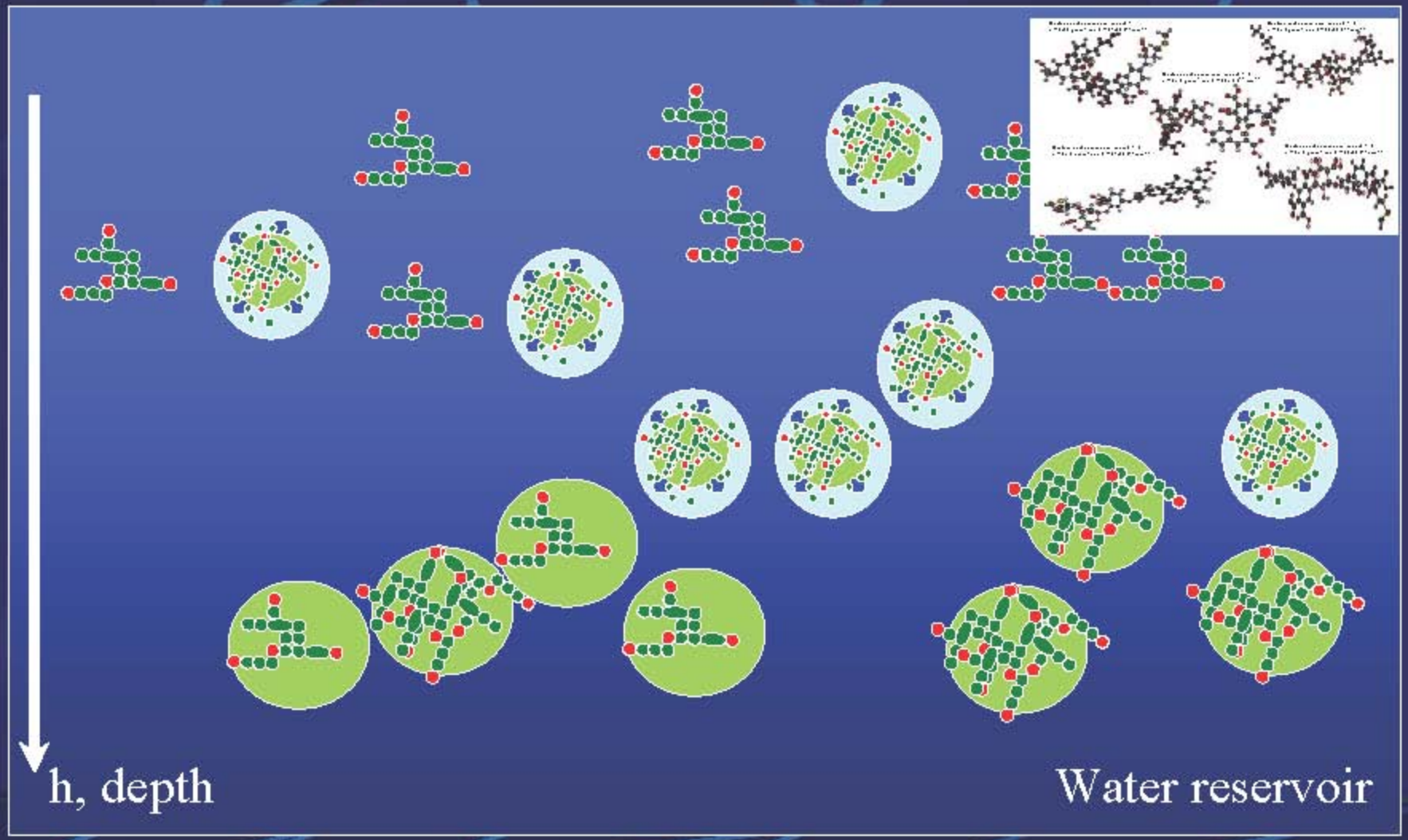
➢ A change in the HS concentration leads to decreasing of red cell aggregation and cell adhesion by emulsion drops only *within the definite interval* of the HS concentration.

3. Quantum statistical model of HS

- Particles and associates of HS in water solution can be described as unique ensemble.
- Particles and associates of HS of unique ensemble have different phase (micro phase) states, such as single molecules, micelles, and coagulants.
- Remediation effect of HS in water is due to micelles

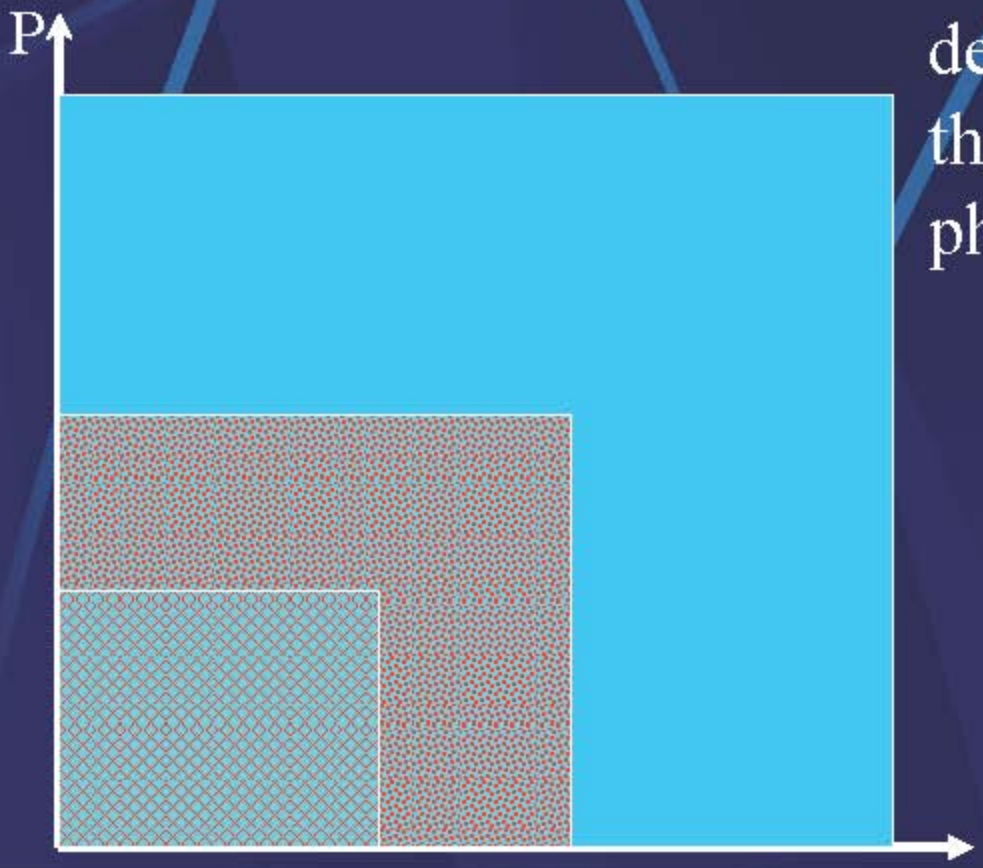
3. Quantum statistical model of HS

❑ Ensemble of HS particles:



3. Quantum statistical model of HS

❑ Quantum statistical approach to substances:



➢ A change in particle description in dependence on the element of considered phase space dΓ:

$$d\Gamma = d\vec{p} \cdot d\vec{r}$$

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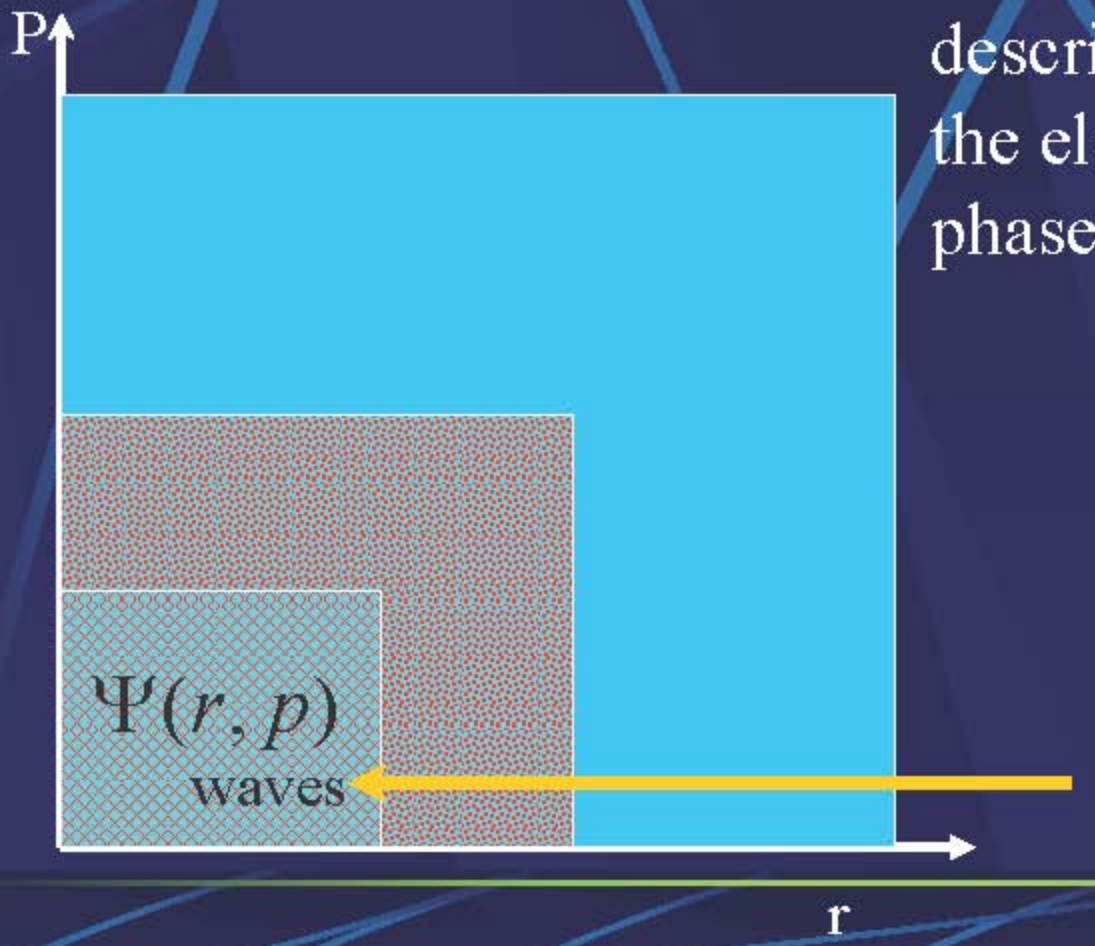

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Quantum mechanical description

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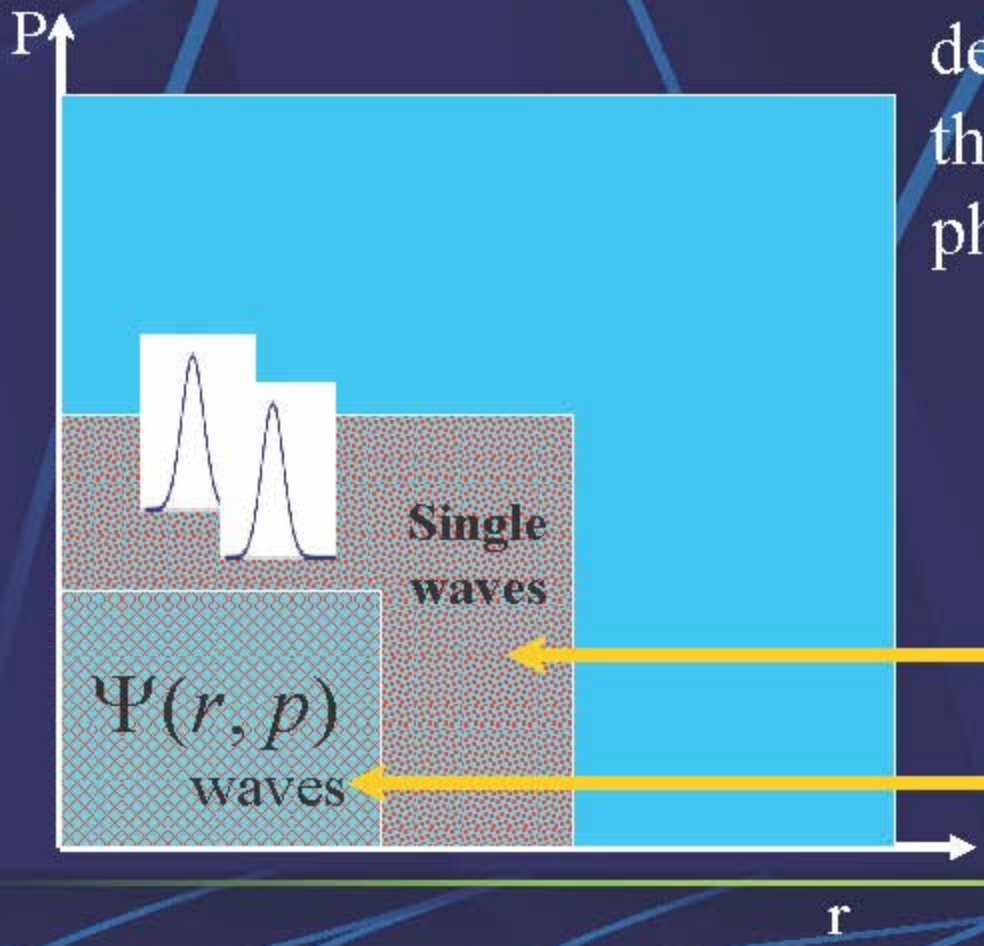

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Quasi-classical approximation

Quantum mechanical description

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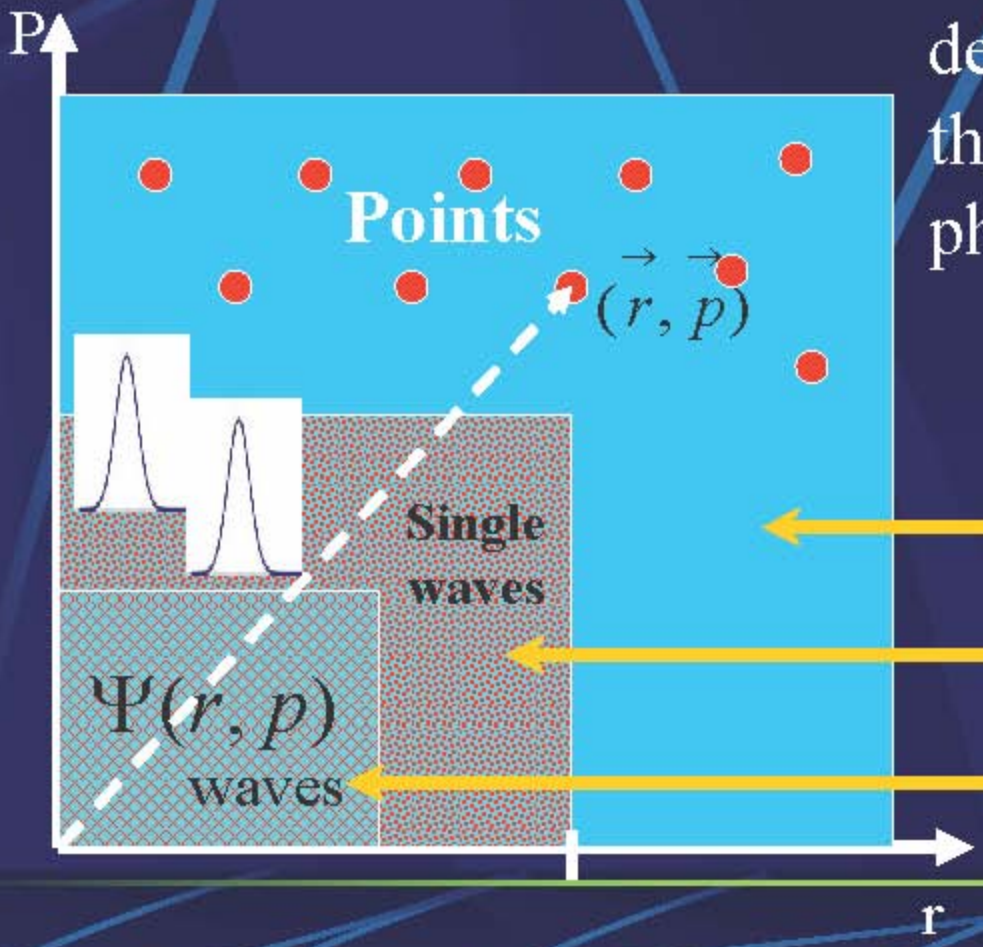

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Classical description

Quasi-classical approximation

Quantum mechanical description

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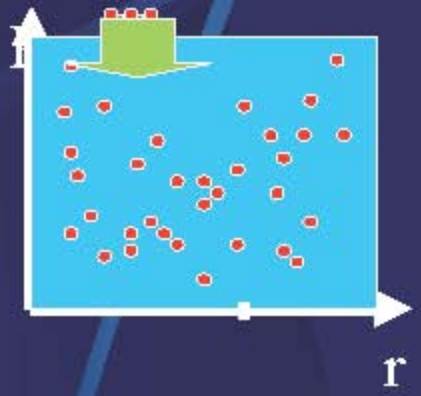
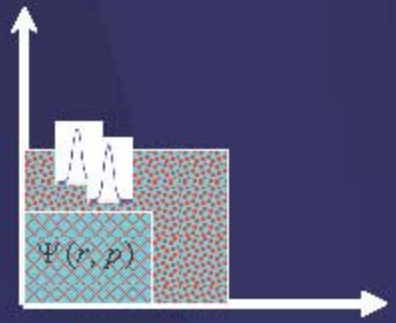


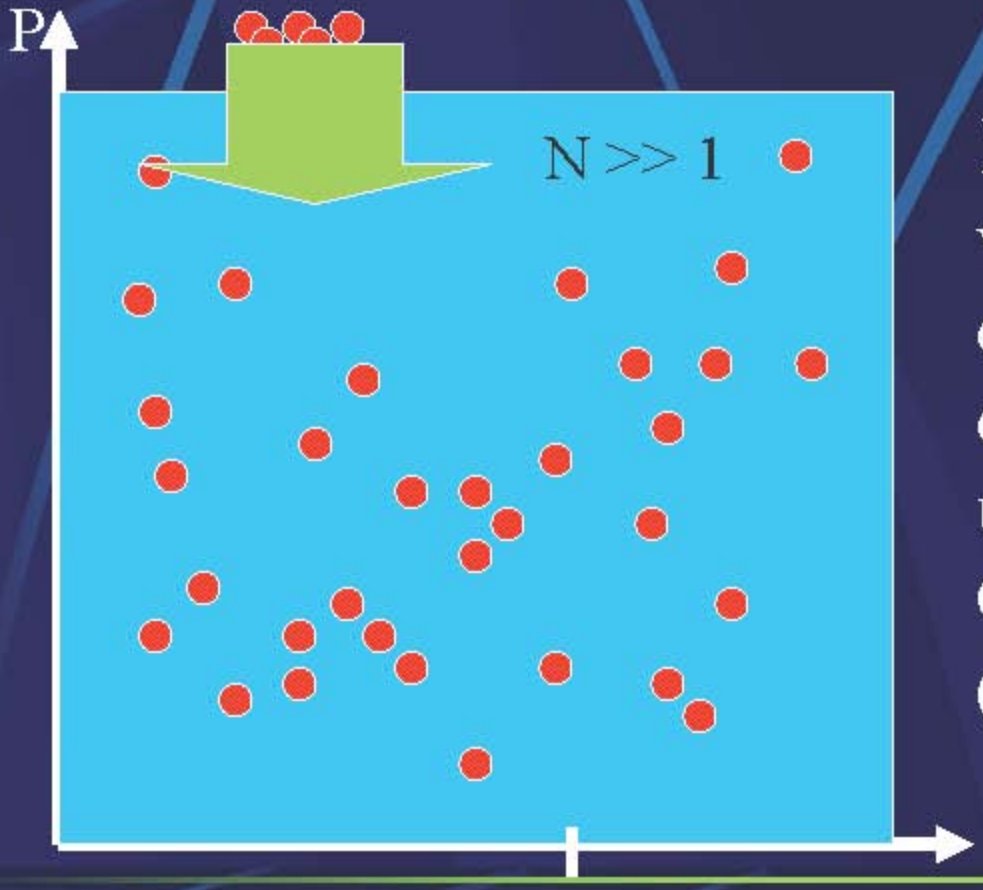
Gibbs formalism to describe a statistical ensemble of HS particles



A Fermi – Dirac statistics to describe protons in HS

3. Quantum statistical model of HS

❑ Description of an ensemble of HS particles (Gibbs formalism):



➢ A statistical ensemble with changeable number of particles N can be described using grand canonical Gibbs distribution/ (T - μ) - distribution

3. Quantum statistical model of HS

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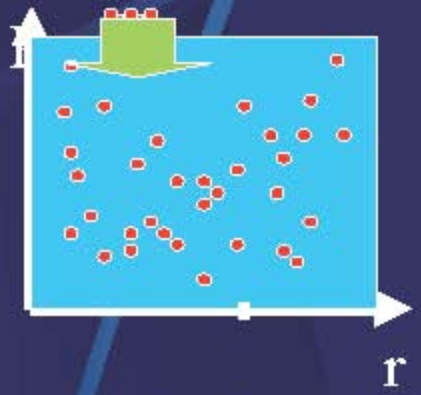

➢ The distribution of ensemble particles including molecules, micelles, and coagulants within the phase space

$$\Delta \vec{q}_{macro} \cdot \Delta \vec{p}_{all}$$

can be described with a probability measure of the grand canonical coordinates

$$\rho\left(\vec{q}, \vec{p}\right) \cdot d\vec{q} \cdot d\vec{p}$$

$\vec{q}$ and $\vec{p}$:

$$\int_{\Delta \vec{q}_{macro}} \int_{\Delta \vec{p}_{all}} \rho\left(\vec{q}, p\right) \cdot d\vec{p}\, d\vec{q} = 1$$

3. Quantum statistical model of HS

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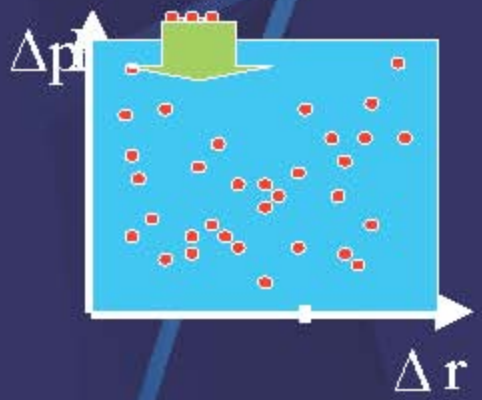

➢ Taking into account a large size and mass of particulate HS, and correspondingly, their high value of inertness, a micro-phase space can be written as follows:

$$d\vec{q}\cdot d\vec{p}$$

$$d\vec{q}\cdot(\vec{v}_{av}\cdot dm_{\mathrm{HS}})$$

$$dq\cdot dp = dq\cdot(4\pi\cdot m_{HS}^{2}\cdot v_{av}^{3}\cdot dm_{\mathrm{HS}})$$

• an averaged velocity of HS particles within Δr

$$J_{P} = \int_{\Delta q_{macro}} \rho(q,p)\cdot dq \quad \Rightarrow \quad f(m_{HS})$$

3. Quantum statistical model of HS

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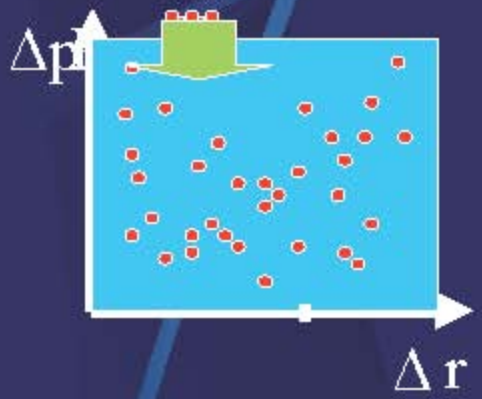

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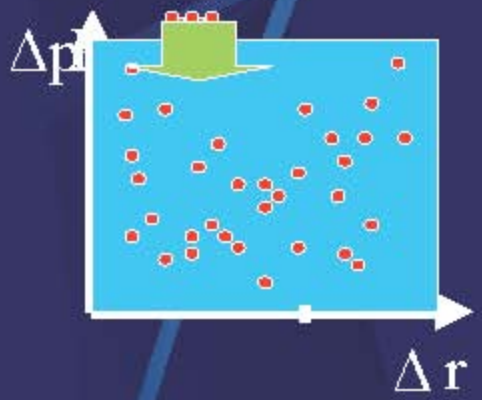

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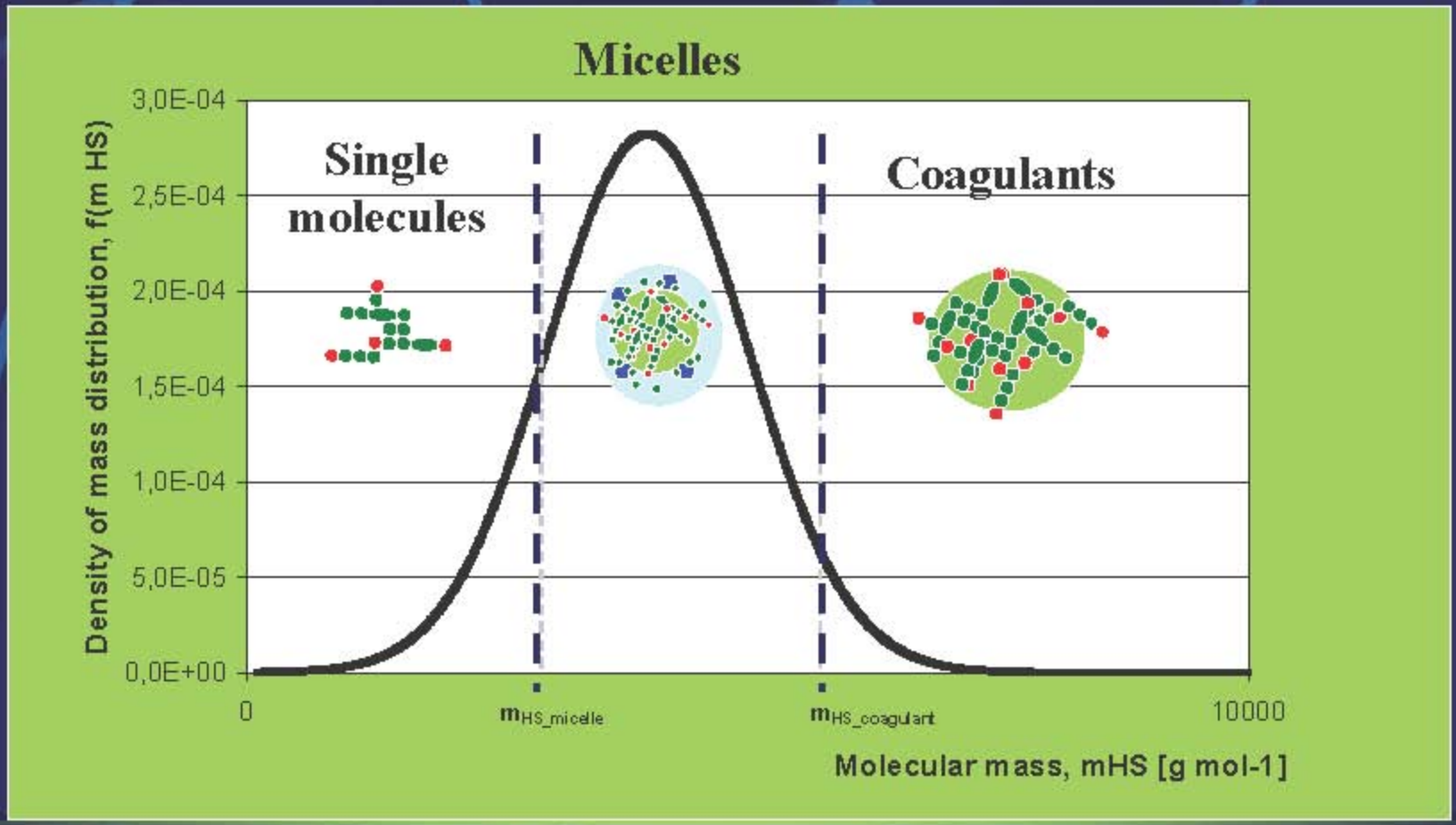
$$f(m_{HS})$$

$$\int_{\Delta m_{HS}} f(m_{HS})\cdot dm_{HS} = 1$$

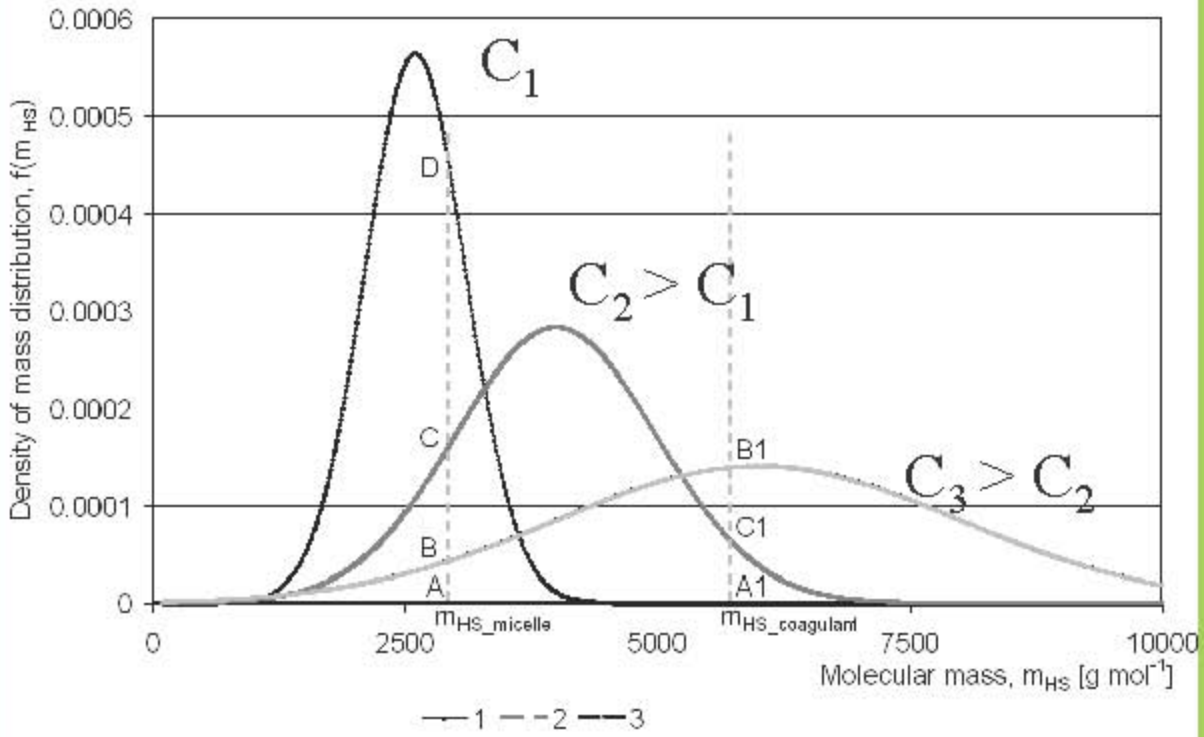
3. Quantum statistical model of HS

❑ Gibbs distribution and an ensemble of HS particles:



3. Quantum statistical model of HS

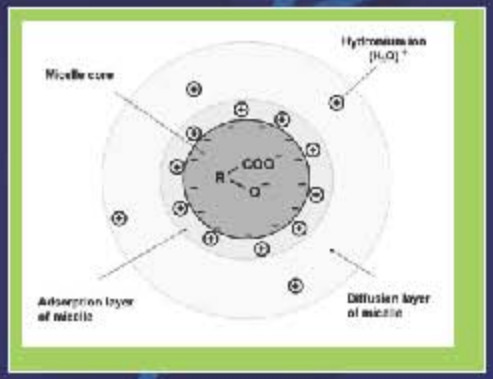
❑ Gibbs distribution at different HS concentrations



➢ Increase in HS concentration first results in an increasing of the micelle portion, and then, its decrease.

3. Quantum statistical model of HS

❑ Particularities of micelles:



- Micelle is a charged particle.

(Usually, negatively charged)

- It is formed from HS molecule when its mass exceeds the critical value $m_{HS\_micelle}$.
- As a result, micelles contains a lot of contaminants inside of it. Therefore, contaminants become not available for the environment.

3. Quantum statistical model of HS

❑ Particularities of micelles:

Hypothesis:

- In activity of HS paramagnetic centers, protons play substantial role.
- Proton is a Fermi particle with s=1/2. It poses paramagnetic properties: $\mu_p = 2.793\ \mu_N$.

Magnetic interaction of proton with magnetic field of electrons of functional group (-OH; -COOH) leads to hyperfine structure of energetic level E_p of proton that becomes not generate in a weak external magnetic field produced by other functional group

3. Quantum statistical model of HS

❑ Particularities of micelles:

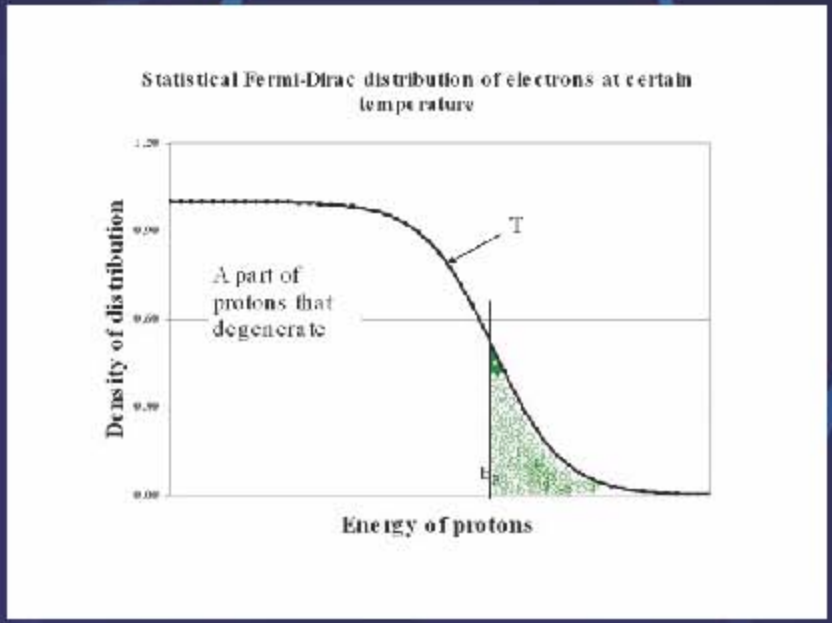
Magnetic interaction of proton with magnetic field of electrons of functional group (-OH; -COOH) leads to hyperfine structure of energetic level E_p of proton that becomes not generate in a weak external magnetic field produced by other functional group

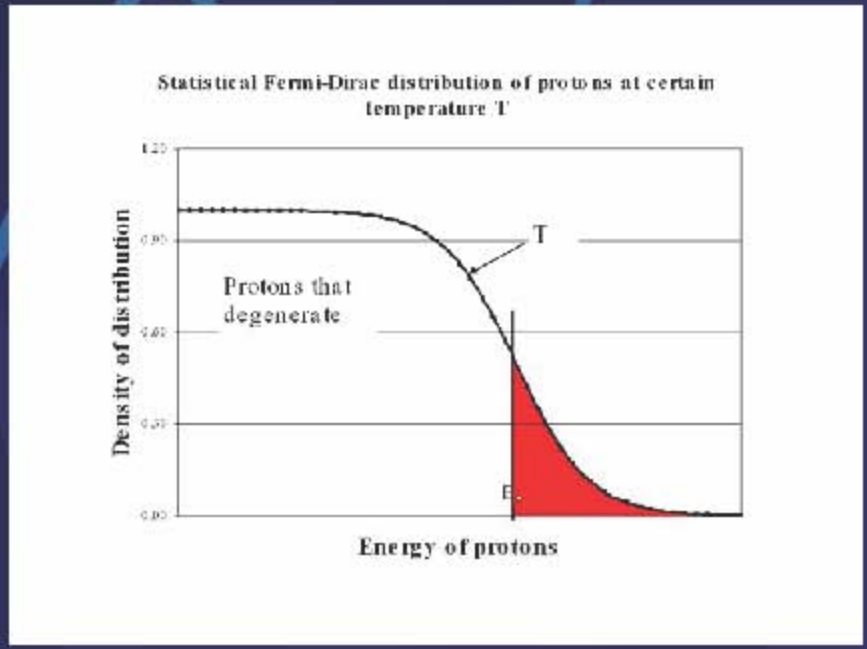
A significant spatial shift of proton in its functional group relative core of functional group and a shift between centers of distributions of negative and positive charges

Some protons become substantially excited, can magnetically and electrically interact with another functional group, and can become movable.

3. Quantum statistical model of HS

❑ Particularities of micelles:



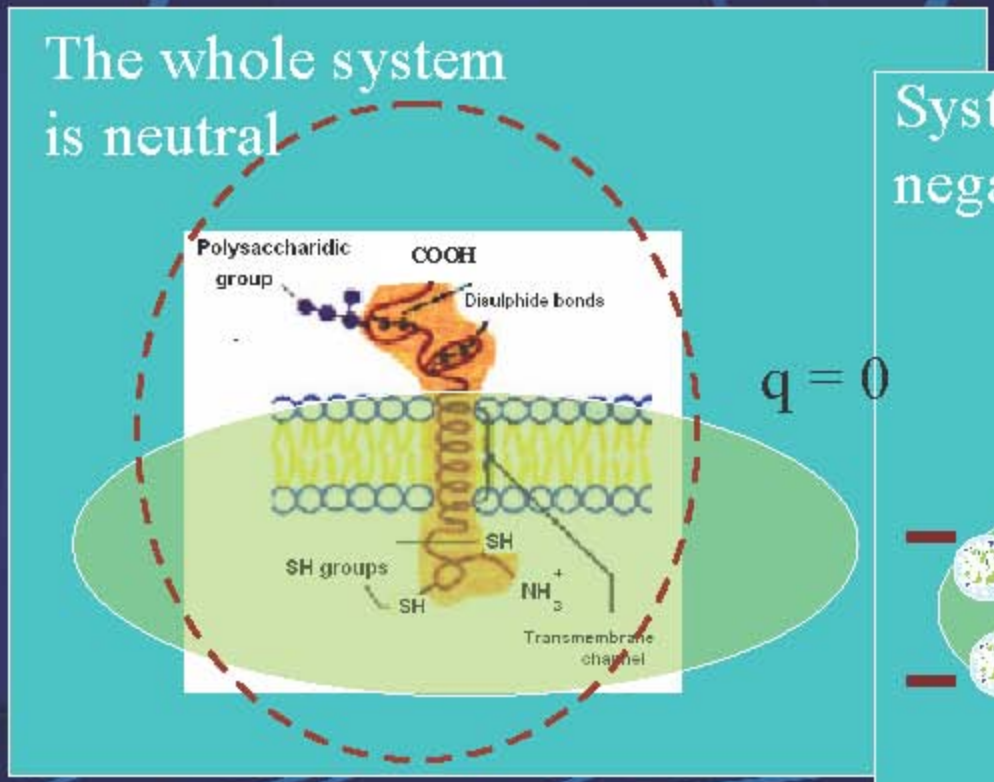


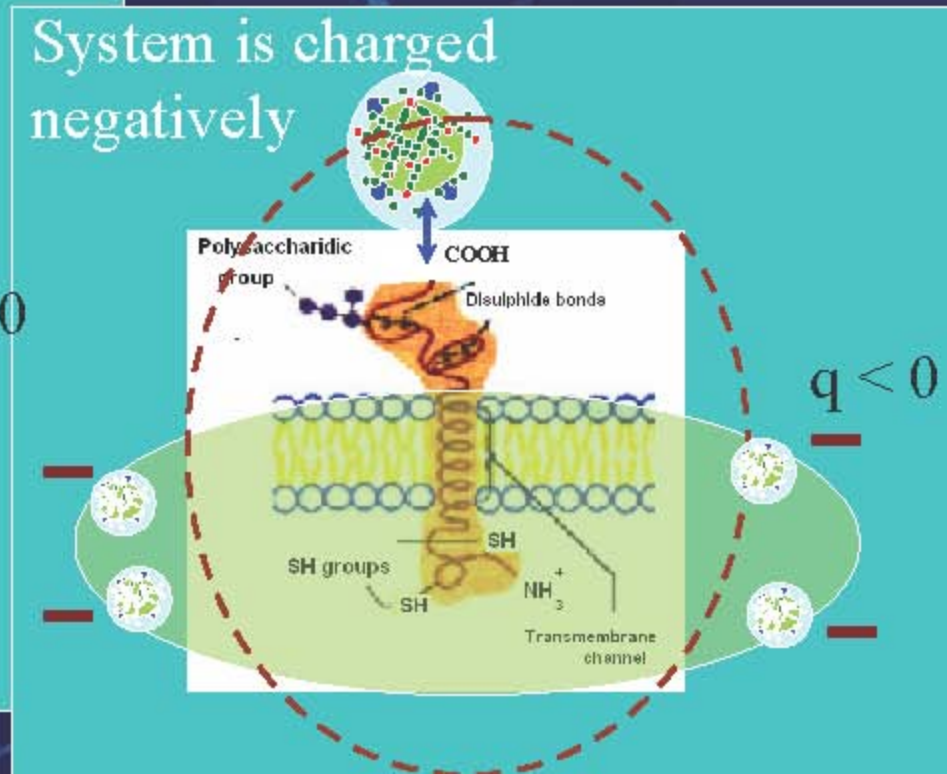
electrons

protons

4. Application of presented concept to remediation effect of HS

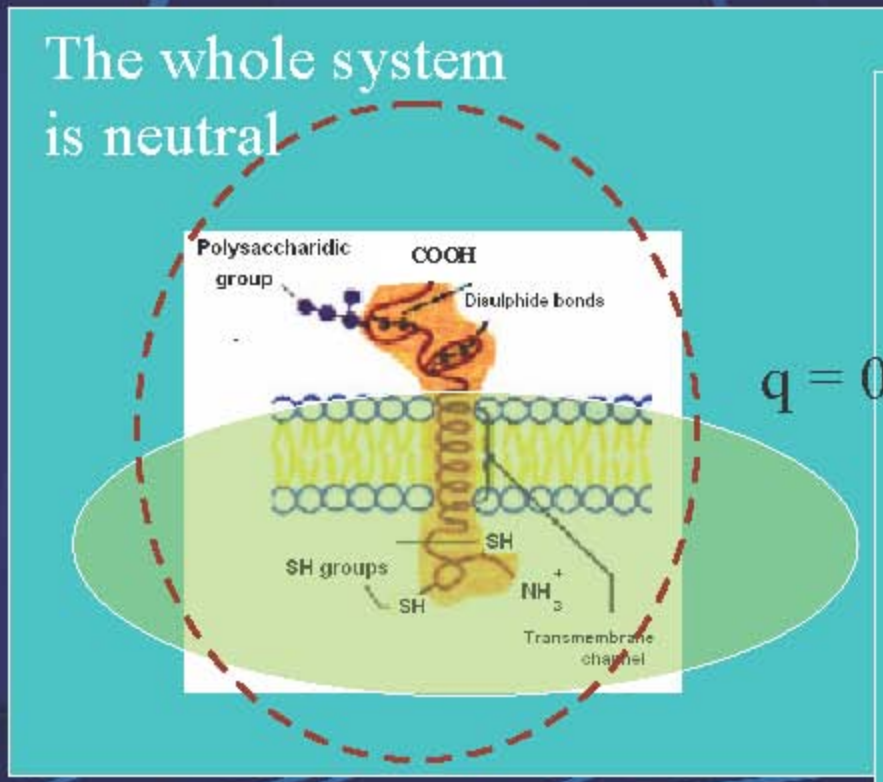
- Micelles interact with neutral or slightly charged cells via movable protons, being bound to functional units of protein of cell membrane

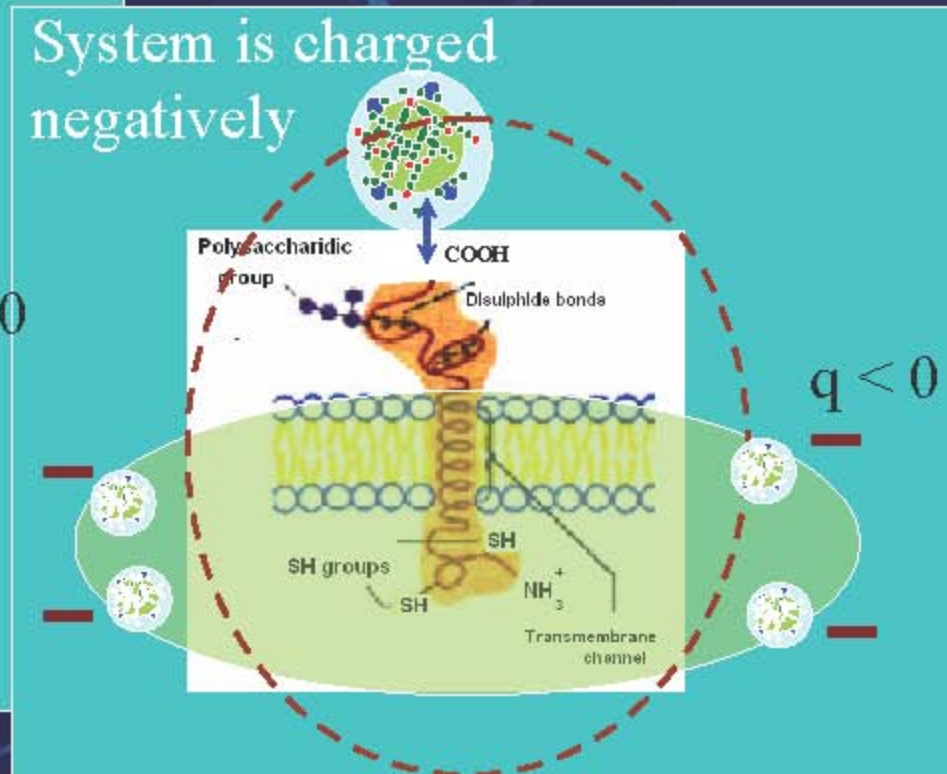




4. Application of presented concept to remediation effect of HS

- Optimal concentration of micelles are observed only within the definite interval of HS concentration in water solution.





5. Conclusions

- The proposed quantum statistical model of HS allows for understanding physical, chemical, and biomolecular processes with mediating role of HS.
- Model based on (1) quantum statistical approach to statistical system with a great changeable number of particles, and (2) paramagnetic properties of protons, allows for interpreting reduction of red cell aggregation in blood, adding of HS to blood.

Thank you for your attention