

# A SIMPLE APPLICATION OF F.I.R.M. METHOD

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This talk addresses the question of aerosol depletion on sea water surfaces providing an illustration of a more general model developed for the so called FIRM systems, so to say Finely, Intricate, Random Multiphase systems [1], [2]. References: last slide.

An equivalent method was applied a few years ago for airborne particle deposition on canopy forests see [3], [4] air water systems [5].

FIRM systems are characterized by several phase domains broken up in a lot of distinct space domains having complex geometrical shapes. Furthermore, these phase domains change with time or/and randomly.



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STARTING from balance equations for exact local instantaneous quantities such as the airborne particle concentrations  $\gamma_k$  in rough or smooth domains defined by their phase index  $\alpha_k$  functions with their boundary conditions on the phase interfaces. DERIVE balance equations for global quantities  $\tilde{\gamma}_k = \langle \overline{\alpha_k \gamma_k} \rangle$  defined available at any point and time. METHOD a weighting operation  $\langle \bar{\bullet} \rangle$  involving time and space integration plus a probability mean in addition with a surface density distribution  $\sigma^s$  produce volumetric source terms in the equations for  $\tilde{\gamma}_k$  from the interface interactions within phases. Let us consider phase space domain  $\Omega$  defined by a surface f. The velocity  $\vec{V}$  of a surface point satisfies  $\frac{\partial f}{\partial t} = -\vec{V} \cdot \vec{\nabla} f$ . A surface density is defined by  $\sigma^s = -\delta(f) \cdot \|\vec{\nabla} f\|$ . The  $\alpha$  phase index is :  $\alpha(\vec{M},t) = H[f(\vec{M},t)]$ . So  $\frac{\partial \alpha}{\partial t} = -\delta(f)\vec{V} \cdot \vec{\nabla} f$  and  $\vec{\nabla}\alpha = \delta(f)\vec{\nabla}f.$ 

Using the surface density these two derivatives can be rewritten as quantities related to a volume:  $\frac{\partial \alpha}{\partial t} = \sigma \vec{n} \cdot \vec{V}$  and  $\vec{\nabla} \alpha = -\sigma \vec{n}$ . These relations allow transforming conditions on surfaces to source terms in volumes.





## A SIMPLE APPLICATION TO AIR-OCEAN AEROSOL DEPOSITION

Let us consider aerosol deposition on the ocean (or atmosphere water systems).

We identify three phases: water, atmosphere above rough water surfaces and the one above smooth parts. The rough phase  $\Omega_R(t)$ , with its index  $\alpha_R$ , is a set  $N_R$  subdomains  $\Omega_{Rm}$  with index  $\alpha_{Rm}$ . Within each of them we have an interface with the smooth phase  $\partial \Omega_{Rm,S}(t)$ , a water surface and water drop inclusions, so  $N_{Rm,W}(t)$  water phase subdomain surfaces  $\partial \Omega_{Rm,Wi}(t)$  so we write:  $\partial \Omega_{Rm} = \partial \Omega_{Rm,S}(t) + \sum_{i=1}^{N_{Rm,W}(t)} \partial \Omega_{Rm,Wi}(t)$  and  $\partial \Omega_R = \sum_{m=1}^{N_R} \partial \Omega_{Rm}(t)$ .



Index derivatives have nonzero values only if the considered point is located on one of the phase interfaces at a given time. So we can write rough subdomain index derivatives as a sum:

(1) 
$$\frac{\partial \alpha_{Rm}}{\partial t} = \sigma_{Rm,L} \vec{n}_{Rm,L} \cdot \vec{V}_{Rm,L} + \sum_{i=1}^{N_{Rm,W}(t)} \sigma_{Rm,Li} \vec{n}_{Rm,Li} \cdot \vec{V}_{Rm,Li} \text{ and } \frac{\partial \alpha_{R}}{\partial t} = \sum_{m=1}^{N_{R}} \frac{\partial \alpha_{Rm}}{\partial t}$$
  
(2)  $\vec{\nabla} \alpha_{Rm} = -\sigma_{Rm,L} \vec{n}_{Rm,L} + \sum_{i=1}^{N_{Rm,W}(t)} \sigma_{Rm,Li} \vec{n}_{Rm,Li} \text{ and } \vec{\nabla} \alpha_{R} = \sum_{m=1}^{N_{R}} \vec{\nabla} \alpha_{Rm}$ 

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# BALANCE EQUATION FOR WEIGTHED CONCENTRATION $\tilde{\gamma}_{R}$ .

Basic aerosol instantaneous balance equation for within the rough or the smooth phase

is (3)  $\frac{\partial \gamma_R}{\partial t} + \vec{\nabla} \cdot \vec{j}_R = 0$  where  $\vec{j}_R$  stands for the resulting aerosol deposition processes in the considered

phase. We intend to derive a balance equation for  $\tilde{\gamma}_R = \langle \overline{\alpha_R \gamma_R} \rangle$ . Multiplying (3) by  $\alpha_R$ , applying a weighting operation and taking advantage of its properties we obtain :

(4) 
$$\frac{\partial \tilde{\gamma}_R}{\partial t} + \vec{\nabla} \cdot \tilde{\vec{j}}_R = \overline{\left\langle \gamma_R \frac{\partial \alpha_R}{\partial t} + \vec{j} \cdot \vec{\nabla} \alpha_R \right\rangle}$$

The source term on the right hand side can be rewritten with the relation (1) and (2) and we obtain for rough and smooth phases:

( )

(5) 
$$\frac{\partial \tilde{\gamma}_{R}}{\partial t} + \vec{\nabla} \cdot \tilde{\vec{j}}_{R} = \Gamma_{RW} + \Gamma_{RS} \\ \frac{\partial \tilde{\gamma}_{S}}{\partial t} + \vec{\nabla} \cdot \tilde{\vec{j}}_{S} = \Gamma_{SW} - \Gamma_{RS} \end{cases}$$
(6) 
$$\Gamma_{RW} = \left\langle \sum_{m=1}^{N_{R}} \sum_{i=1}^{N_{Rm,W}(t)} \sigma_{Rm,Li} \left( \gamma_{R} \vec{V}_{Rm,Wi} - \vec{j}_{R} \right) \vec{n}_{Rm,Wi} \right\rangle$$
$$\Gamma_{RS} = \overline{\left\langle \sum_{m=1}^{N_{R}} \sigma_{Rm,S} \left( \gamma_{R} \vec{V}_{Rm,S} - \vec{j}_{R} \right) \vec{n}_{Rm,S} \right\rangle} = -\Gamma_{SR}$$
$$\Gamma_{SW} = \overline{\left\langle \sum_{m=1}^{N_{S}} \sigma_{Sm,W} \left( \gamma_{S} \vec{V}_{Sm,W} - \vec{j}_{S} \right) \vec{n}_{Sm,W} \right\rangle}$$





One specific deposition process q on water within a phase k is  $\Gamma_{kWq} = -\sigma_{kWq}V_qc_k$  where  $\sigma_{kWq}$  is the surface density for process q,  $V_q$  deposition velocity and  $c_k$ 

concentration in the phase  $c_k = \frac{\tilde{\gamma}_k}{\tilde{\alpha}}$ .

For the smooth and rough phases:  $\Gamma_{SW} = -\sum_{q} \Gamma_{kWq} = -\sigma_{SW} V_S c_S \quad \Gamma_{RW} = -\sum_{p} \Gamma_{kWqq} = -\sigma_{RW} V_R c_R$  Without deposition in the transfer area and assuming that the integral can be approximated :

$$-V_T \gamma_{ref} = \int_0^{\delta} (\Gamma_{SW} + \Gamma_{RW}) dz \quad (8) \quad V_T = a_S V_L \frac{\tilde{\alpha}_S c_S(\delta)}{\gamma_{ref}} + a_R V_{ER} \frac{\tilde{\alpha}_R c_R(\delta)}{\gamma_{ref}}$$
  
where  $a_{kq} = \frac{A \delta \sigma_{kWq}}{A_k}$  is a wave index defined as the deposit  
surface for process  $q$  in phase  $k$  by its unit of horizontal  
surface and  $a_k V_k = \sum_q a_{kq} V_q$ 

Therefore, we have to solve (7) to obtain  $c_s(\delta)$  and  $c_R(\delta)$  and find the deposition velocity  $V_T$  at the reference height through (8).



Solutions are built as

$$\frac{d}{dz} \left[ \tilde{\alpha}_{S} D_{S} \left( z \right) \frac{dc_{S}}{dz} \right] = -\sigma_{LR} V_{h} \left( c_{R} - c_{S} \right)$$

$$\frac{d}{dz} \left[ \tilde{\alpha}_{R} D_{R} \left( z \right) \frac{dc_{R}}{dz} \right] = \sigma_{LR} V_{h} \left( c_{R} - c_{S} \right)$$

has to be solved.

$$c_{R} = f(z) - \frac{g(u(z))}{\tilde{\alpha}_{R}u_{R}^{*}}$$

$$c_{S} = f(z) + \frac{g(u(z))}{\tilde{\alpha}_{S}u_{S}^{*}} \qquad \theta = 2 \left[ z_{ref} \sigma_{LR}V_{h} \frac{\sum_{\lambda \in A} \tilde{\alpha}_{k}u_{k}^{*}}{\lambda \tilde{\alpha}_{R} \tilde{\alpha}_{L}u_{R}^{*}u_{L}^{*}} \right]^{\frac{1}{2}}$$

$$u(z) = \theta \sqrt{\frac{z}{z_{ref}}}$$

Boundary conditions and hypotheses for turbulent diffusion

for 
$$z = z_{ref}$$
  $\forall z \ge z_{r_{ref}}$   $\tilde{\gamma}_k = \langle \alpha_k \gamma \rangle \rightarrow \langle \alpha_k \rangle \gamma_{ref} = \tilde{\alpha}_k \gamma_{ref}$   
 $\tilde{\gamma}_S \rightarrow \tilde{\alpha}_S \gamma_{ref}$   $\tilde{\gamma}_R \rightarrow \tilde{\alpha}_R \gamma_{ref}$   $c_S \rightarrow \gamma_{ref}$   $c_R \rightarrow \gamma_{ref}$ 

for 
$$\overline{z = \delta}$$
  $D_k \frac{dc_k}{dz}\Big|_{z=\delta} = a_k V_{Ek} c_{\delta k}$  where settling is

ignored.

<u>Turbulent diffusion</u> inside phase:  $D_k(z) = \lambda u_k^* z$   $\lambda = 0.41$ 

<u>Smooth Rough Exchanges</u> :  $\Gamma_{SR} = \sigma_{SR}V_H(c_R - c_S)$  with  $\sigma_{SR}$  smooth-rough exchange interface amount by unit of volume,  $V_H$  horizontal transfer velocity.

where it appears a coupling factor  $\theta$ . With the previous elements, (9) is turn into a Bessel hyperbolic equation with a general solution based on modified Bessel functions of first and second kind :

$$g(z) = C_1 I_0 \left(\theta \sqrt{\frac{z}{z_{ref}}}\right) + C_2 K_0 \left(\theta \sqrt{\frac{z}{z_{ref}}}\right)$$



The boundary conditions provide the 2 constants and the solution is:

$$u_{z} = \theta \sqrt{\frac{z}{z_{ref}}} \quad u_{\delta} = \theta \sqrt{\frac{\delta}{z_{ref}}} \quad A(z) = \frac{2\left[I_{0}\left(u_{z}\right)K_{0}\left(\theta\right) - K_{0}\left(u_{z}\right)I_{0}\left(\theta\right)\right]}{u_{\delta}\left[I_{0}\left(\theta\right)K_{1}\left(u_{\delta}\right) + I_{1}\left(u_{\delta}\right)K_{0}\left(\theta\right)\right]} \quad \left[10$$

$$\frac{c_{R}\left(z\right)}{\gamma_{ref}} = 1 + \frac{1}{\Delta}\left[\left(\sum \tilde{\alpha}_{k}u_{k}^{*}X_{k} + X_{S}X_{R}A_{\delta}\sum \tilde{\alpha}_{k}u_{k}^{*}\right)ln\left(\frac{z}{z_{ref}}\right) - \tilde{\alpha}_{S}u_{S}^{*}\left(X_{S} - X_{R}\right)A(z)\right] \quad \left[\Delta = \tilde{\alpha}_{S}u_{S}^{*}\left(1 + X_{S}\ln_{\delta}\right)\left(1 + X_{R}A_{\delta}\right) + \tilde{\alpha}_{R}u_{R}^{*}\left(1 + X_{R}\ln_{\delta}\right)\left(1 + X_{S}A_{\delta}\right)\right] \quad X_{k} = \frac{a_{k}V_{Ek}}{\lambda u_{k}^{*}} \quad V_{T} = \frac{\lambda \sum \tilde{\alpha}_{k}u_{k}^{*}X_{k} + X_{S}X_{R}A_{\delta}\sum \tilde{\alpha}_{k}u_{k}^{*}X_{k} + X_{S}X_{R}A_{\delta}\sum \tilde{\alpha}_{k}u_{k}^{*}\right] + \tilde{\alpha}_{R}u_{R}^{*}\left(X_{S} - X_{R}\right)A(z)$$

The main parameters of the problem are

 $1//// \alpha_k u_k^*$ : friction velocity weighted by the phase size. These parameters are related to the vertical transfer of airborne particles to the liquid surfaces where their deposit takes place.

$$2///\frac{\delta}{z_{raf}}$$
: ratio of the deposition height to the location where the concentration is constant.

3///  $X_s$  et  $X_R$  : ratio which compares the deposit velocity weighted by the wave index  $a_k V_{Ek}$  with the friction velocity  $u_k^*$ .

4////  $\theta$  gives a measure of the horizontal exchanges between the smooth and rough phases.



Two limit cases can be easily understood for the total deposition velocity  $V_T$  at the reference height  $z_{ref}$ 

depending of the ratio of the deposition velocity to friction velocity :  $X_k = \frac{a_k V_{Ek}}{\lambda u_k^*}$ :

 $\mathbf{A}$ If  $X_s$  et  $X_R$  are small enough,  $\Delta \rightarrow \sum \tilde{\alpha}_k u_k^*$  and  $V_T \rightarrow \lambda \sum \tilde{\alpha}_k u_k^* X_k = \sum \tilde{\alpha}_k a_k V_k$ 

 $V_T$  is just the sum of the deposition velocities of the smooth and rough phases weighted by their relative magnitude. There is roughly no exchange within the phases because the deposits in both phases are small enough to be supplied by its own vertical transfer

### B

If  $X_s$  et  $X_R$  are big enough,  $\Delta \to X_s X_R A_\delta \ln_\delta \sum \tilde{\alpha}_k u_k^*$  and  $V_T \to \frac{\lambda}{\ln_\delta} \sum \tilde{\alpha}_k u_k^*$ .

In this case the diffusion process in the vertical transfer cannot supply enough particles for feeding a big deposition velocity on the liquid surfaces. Therefore, the total deposition velocity  $V_T$  is associated with the vertical transfer possibilities and limited by turbulence intensities.



For a parametric study, relations **10** are written down in Microsoft Excel program. Hereafter an illustration of a case where all parameters are identical except the coupling factor which takes two values: 0 and 10. So to say, without and with aerosol exchanges from smooth to rough phases



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Thank You For Your Attention

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