

MULTI-DOMAIN PARALLEL MATHEMATICAL MODEL TO EVALUATE THE ENVIRONMENTAL IMPACT OF SOLID WASTE DISPOSAL IN THE SOIL

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Abstract: *The urban solid waste management system in Brazil has the landfill as an economical solution for the final destination. However, the organic matter decomposition mechanism is a relevant aspect that not was completely explored yet. This work aims to compare two mathematical models that evaluate the inorganic ions diffusion and sorption phenomenon and show the computation performance for different cluster and domain configurations. The code validation was carried out by comparison of experimental data obtained in laboratory and field tests. The multi-domain parallel version of the code was constructed using the MPI routines for processors communications. The results showed that the inorganic ions migration process can not be explained completely as result of diffusion, but also by the mass transfer phenomenon of contaminant species and the interstitial liquid of the soil to the own soil particle and vice-versa. It was obtained a super linear speed up behavior for the multi-domain parallel code performance for almost all computations, except when observed a bad loading balance and high network traffic.*

Key words: *Solid waste, Diffusion, Sorption, Mass transfer, Parallel computing*

1. INTRODUCTION

The landfill technique is largely used in the world as an economically suitable solution for the final solid waste disposal due to the feasibility in implementation and operation which requires less investment if compared to alternatives such as incineration, selective collection and composting plants. The leached is generated by the solid waste degradation process and by the rain water passing in the porous environment (soil). The urban solid waste continuously accumulated is not inactive because it consisting in a several chemical species influenced by nature agents (Teixeira et al., 2000).

Several works has been aimed to reproduce the soil contaminant phenomenon by laboratory test (Ritter and Campos, 2006; Rowe et al., 1988) where it is performed in a laboratory cell composed by soil sample and leached. Results proved that the contaminant transport process in the landfill soils is performed by ions sorption and diffusion mechanism from leached to the soil.

In spite of laboratory tests being efficient and reproduce faithfully the phenomena, it can become expensive and takes long time to be carried out. Therefore, as consequence of the development of efficient numerical methods and computers, the mathematical modeling task has become possible and has contributed to increase the understandings generating additional contributions.

Normally the chemical species diffusion analysis is traditionally performed by two methods: analytical and numerical ones. Although analytical methods are more elegant, they require a series of considerations that usually leads to considerable simplifications on the physical phenomena and unrealistic results may arise. Hence, the numerical methods have been used by the scientific community where the finite volume technique (Forster, 2006 and Pinto, 2008) is largely applied to solve the species transport equation.

In order to improve the performance of computational simulation, continuous changes have been observed in a computing platform paradigm for scientific applications. In the past, the scientific computation was performed in large computers with shared memory or in common sequential computer (Vatsa and Hammond, 1998). However, the technological development and the commercial availability of powerful personal computers economically accessible that allow connection with fast communication network created a perfect scenario to build up cluster of computers as an alternative to the large ones (Simões et al., 2005). As consequence of low price, easy maintenance and powerful

processors the clusters of personal computers are becoming popular among scientific computational groups. This architecture offers collective memory to solve scientific complex problems (Vatsa and Wedan, 1999). Although the availability of computer distributed platform has allowed the cluster of computers being an alternative for the supercomputers, this technological advance has changed the rules for code development (Sikora et al., 1998), which needs to be adapted or implemented in distributed machine.

Computing distributed systems are ideally suitable for problems that can be divided into small problems with common boundaries. Most codes developed to solve heat transfer and fluid flow problems demand high memory amount that is available in high performance architecture with distributed memory (Lepper et al., 1997). However for accuracy and consistence reasons a parallel implementation needs exchanges of information after each iteration at the boundaries of sub-domains. This synchronism leads to great amount of data transfer (Hammond, 1997). The communication among computers is carried out utilizing libraries of message passing. The library MPI (Message Passing Interface) has largely been used in the freeware version MPICH (Gropp and Lusk, 1997).

In this work the Rio das Ostras landfill soil was used to compare two mathematical models that evaluated diffusion and sorption phenomena establishing a calculation tool to analyze the environmental impact caused by the solid waste disposal. The computational simulation was carried out by a generic program to solve transport equations set up to environmental problems. This code is called MPHMTM (Multi Phase Heat and Mass Transfer Program) program (Castro, 2000), constructed in Fortran 90/95 language.

In this context, this work presents a multi-domain parallel three dimensional mathematical model able to simulate the solid waste environmental impact in the Rio das Ostras soil with the objective of showing the improvement of performance of the code based on multi-domain parallel technique which allows the simulations with larger memory amount and higher performance computation needs.

2. MATHEMATICAL MODEL

In the model is formulated the contaminants transport phenomena that occur among solid and liquid phases of landfill soil, where it is treated as a system of two phases. The phenomenon of mass transfer in the multiphase flow can be described by the conservation Eq. (1) that expresses the punctual balance of mass.

$$\frac{\partial}{\partial t} (\epsilon_j \rho_j \phi_{ij}) + \text{div} (\epsilon_j \rho_j \bar{U}_j \phi_{ij}) - \text{div} (\epsilon_j D_{ij} \text{grad}(\phi_{ij})) = \dot{S}_{\text{esp}} \quad (1)$$

where ϕ_{ij} is mass fraction of each species in each phase, ϵ_j is the porosity in each phase, ρ_j is the density in each phase, D_{ij} is the diffusion coefficient of each species of each phase, \bar{U}_j represents the phase velocity obtained by solution of momentum equation in the porous environment and the \dot{S}_{esp} is the source term, that in this work was modeled in two different way for forward comparison with experimental data.

According to Valadão (2008) the source term in Eq. (1) is associated to the chemical species sorption by the solid phase. The mass balance among the solid phase and liquid phase considers the solid phase with null velocity and in chemical equilibrium with the liquid phase. The relationship among the contaminant amount adsorbed in the solid phase and the existent amount in equilibrium in the liquid phase is known as sorption isotherm that can be linear or not. The relationship used in laboratory test is that the solution concentration is linearly proportional to the adsorbed amount in the solid phase.

The literature (Perry and Green, 1985) refers to the equilibrium among the liquid concentration in the solid phase and the concentration in the liquid ($\phi \times C$) as sorption isotherm. This equilibrium can be depend of own concentration in the liquid and can be represented in a graphic that do the relation with the solute mass fraction in the particle and the concentration in the liquid phase as pictured in Fig (1).

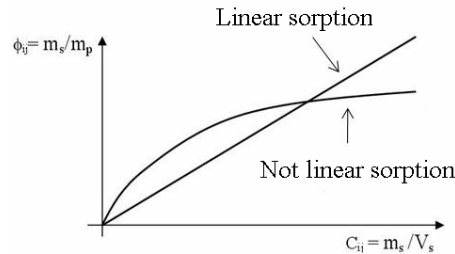


Figure 1. Equilibrium representation among particle solute and the liquid environment (Perry and Green, 1985).

where ϕ_{ij} represents the solute mass fraction in the solid phase, C_{ij} is the concentration in the liquid environment, m_s represents the mass of chemical species present in the liquid phase, m_p is the mass of solid phase and V_s is the volume of liquid solution.

Hence, the distribution coefficient is defined in following way:

$$K_d = \frac{d\phi_{ij}}{dC_{ij}} \quad (2)$$

The source term S_{esp} associated with the chemical species sorption by the solid phase can be null, higher or smaller than zero. When the source term is zero, it does not exist sorption among the liquid and soil. If higher than zero, it means that there is a desorption from soil to the liquid. If negative, it means that there is a species or solute sorption by the soil particles.

The calculation of the source term is modeled with the distribution coefficient definition K_d that describes the equilibrium among the chemical species amount adsorbed by the solid phase and the concentration of the same chemical species in the liquid phase in contact with the particles.

$$[K_d] = \frac{m_s}{m_p} \frac{V_s}{m_s} = \frac{V_s}{m_p} \quad (3)$$

Hence, it is established that:

$$V_s = m_p K_d \quad (4)$$

$$m_s = V_s dC \quad (5)$$

Where it is known that:

$$V_t = V_s \epsilon_s \quad (6)$$

$$\rho_{solid}^{dry} = \frac{m_{particle}^{dry}}{V_{solid}^{dry}} \quad (7)$$

where the term ρ_{solid}^{dry} corresponds to the dry soil density and ϵ_{solid} the porosity of the solid phase.

After the above considerations, the source term can be defined for each chemical species including the distribution coefficient as described below.

$$\dot{S}_{esp} = \frac{m_s}{V_t} \frac{dC}{dt} = \frac{\rho_{solid}^{dry}}{\epsilon_{solid}} K_d \frac{dC}{dt} \quad (8)$$

With the purpose of comparing different methods of source term modeling, Forster (2006) modeled the ion transfer as a function of the mass coefficient transfer β . In this case, the source term is associated with the chemical species mass transfer kinetic by the soil particles as a function of time, described by the following equation.

$$S_{esp} = R_i^L = R_i^S = \frac{dC}{dt} \quad (9)$$

where i corresponds to the chemical species, R_i^L ($\text{kg}/\text{m}^3\text{s}$) is the sorption rate of chemical species by the liquid phase and R_i^S ($\text{kg}/\text{m}^3\text{s}$) is the sorption rate by the solid phase.

The effective contact area among the solid-liquid phase, A_{S-L} , can be determined by the equation:

$$A_{S-L} = \frac{6\epsilon_{soil}}{d_{soil}} \quad (10)$$

where ϵ_{soil} is the soil porosity and d_{soil} (μm) is the particle diameter.

The mass transfer coefficient β (m/s) is given as:

$$\beta_e = \frac{Sh D_i^L}{d_{soil}} \quad (11)$$

where D_i^L is the diffusion coefficient of the chemical species i in the liquid phase (m^2/ano) and Sh is the Sherwood number given by the equation:

$$Sh = 1.17 (Re_{1s})^{0.585} (Sc_i)^{1/3} \quad (12)$$

where Re_{i-s} is the modified Reynolds number among the liquid and solid phases and Sc_i the Schmidt number defined in the following way:

$$Re_{ij} = \frac{\rho_j \varepsilon_i |U_i - U_j| d_j}{\mu_i} \quad (13)$$

$$Sc_i = \frac{\mu_i}{\rho_i D_j^i} \quad (14)$$

ρ is the density of soil grain (kg/m^3), U_i is the species velocity, U_j is the phase velocity, d_j is particle diameter and μ_i is the viscosity species.

Hence, the Eq. (9) can be described according (Richardson and Zaki, 1954; Poirier and Geiger, 1994; Kawasaki et al., 2004):

$$S_{esp} = R_i^L = R_i^S = k \beta_e A_{s-L} \left[\rho_{liquid} \varepsilon_{solid} \right] \left[C_i^{L,S} C_{eq_i}^{L,S} \right]^n v \quad (15)$$

where k is the kinetic constant, $C_i^{L,S}$ is the chemical species concentration in liquid phase in function of time, $C_{eq_i}^{L,S}$ is the chemical species equilibrium concentration in liquid phase contained in the soil interstice, n is the exponent that indicate the equation order and v (m^3) is control volume.

3. SOLUTION SCHEMES

The transport equations were discretized using the Finite Volume Method (FVM) applied for general coordinates system recommended by (Melaen, 1992), where the integration is taken over a control volume as shown in Fig. (2) and Eq. (16). The final product of this operation is an algebraic equation resumed in Eq. (17) and the coefficients obtained by the so-called power law scheme, according Patankar (Patankar, 1980).

$$\iiint \frac{\partial(\rho\varphi)}{\partial t} dvdt + \iint [\text{div}(\rho\vec{U}\varphi) - \Gamma_\varphi \text{grad}(\varphi)] dvdt = \iint S_\varphi dvdt \quad (16)$$

where φ represent the dependent variable, \vec{U} the convective flux and Γ the transport coefficient.

$$a_p \varphi_p = a_w \varphi_w + a_e \varphi_e + a_b \varphi_b + a_t \varphi_t + a_s \varphi_s + a_n \varphi_n + b \quad (17)$$

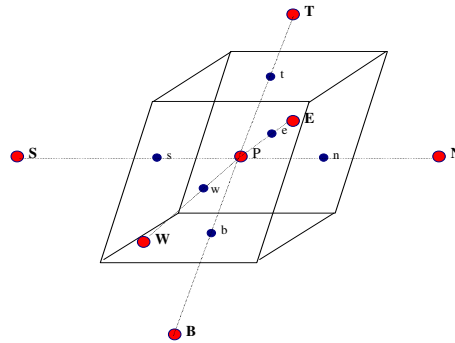


Fig. 2. Control volume

The numerical solution of the algebraic equations resulted from the discretization method demands large computational effort. This code uses the line-by-line method based on the tri-diagonal matrix algorithm (TDMA). The ADI iterative procedure is used within a common solver for all equations.

4. MULTI-DOMAIN PARALLEL CALCULATIONS

This work adopts the parallel technique presented by (Vatsa and Wedan, 1999) that established the distribution of computational load equally among all computers belonging in the process. Particular care was taken during the parallelization process with the domain division algorithm implementation and the parallel routines in order to keep the initial code structure. Aiming at assure good load distribution, it was implemented an algorithm that divided the computational domain and optimally allocates dynamically the memory according to the number of processing node involved in the calculation.

This technique provides that each computing node solves parts of physical domain individually and in addition, besides the computation speed, the number of maximum total control volumes could be linearly increased as the number of processors was increased. Fig. (3) show the physical sub-domain division.

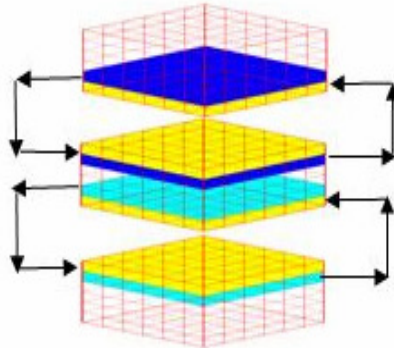


Fig. 3. physical sub-domain division

The division of computational domain establishes domain slice with the same size for each processing node, where these slices can be called of sub-domains. So it is classified for a processing node, with the slaves computers ranked from 1 to n and allowing the number 0 for the master computer, which is in charge of controlling the calculations processes.

The multi-domain parallel technique applied is a MIMD/SIMD (Multiple Instruction Multiple Data)/(Single Instruction Multiple Data), where all computing node, although working individually in an uncouple way, executes equal instruction in the same time due the synchronization process.

In order to guarantee the physical sub-domains solution coupled with the processed information belonging to each boundary sub-domains only the interface data are shared among the sub-domains neighbors for each iteration. For the information exchange among the sub-domains it is necessary a message passing library. The library adopted in this work was the MPI on a freeware version MPICH (Foster et al., 2003). The communication technique adopted among the computers was blocking and standard mode, for both, sends and receives messages that guarantee the synchronism among the computing nodes.

5. RESULTS

The two mathematical model described above were validated through experimental test carry out by (Valadão 2008). The laboratory tests consisted in the chemical species analyses of Rio das Ostras – RJ – Brazil landfill soil. The compacted soil was inserted in a laboratory cell with 9 cm of height and 10 cm of diameter where the initial 3.125 cm was set up as liquid phase (leached), as can be viewed in Fig. (4).

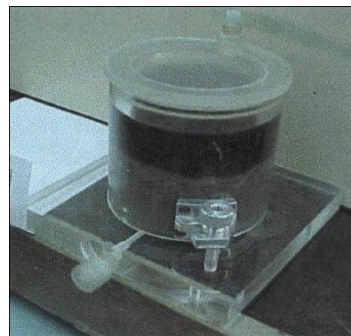


Figure 4. Laboratory cell with soil and leached (Forster, 2006).

The molecular diffusion profile is presented below for the chloride and ammonium ion exists in the leached. In the Fig. (5) and (6) the dotted blue line reproduces the sorption model, the red line represents the kinetic model while the black dot is the experimental values.

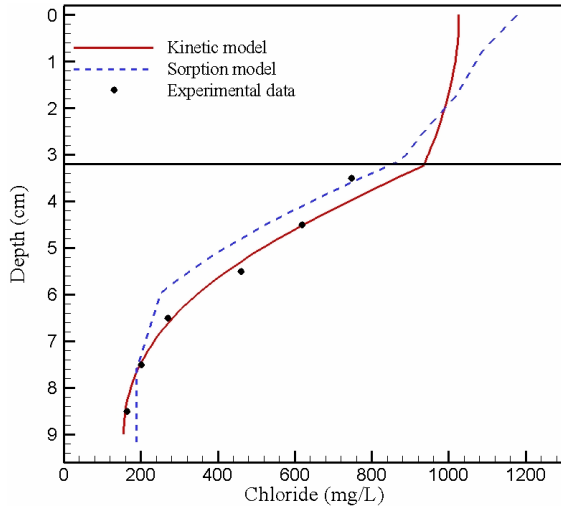


Figure 5. Chloride molecular diffusion profile

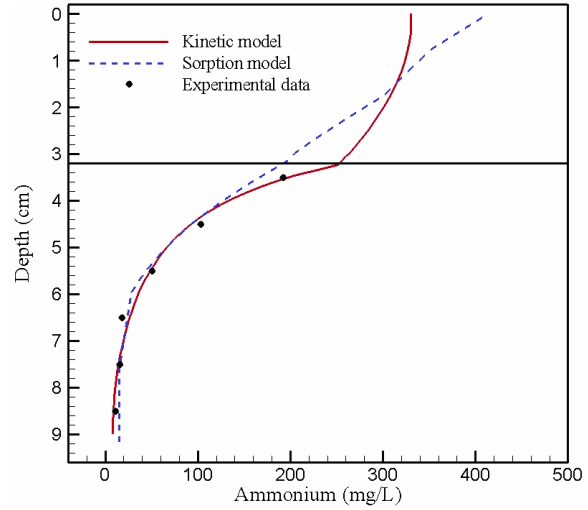


Figure 6. Ammonium molecular diffusion profile

As can be observed in the Fig. (5) and (6), both models can represent the chloride and ammonium molecular diffusion profile. Instead of sorption model has a good approaching to the experimental data, the kinetic model could be better adjusted by the constant kinetic k and by the equation order n . Hence, the kinetic model achieved reproduces more faithfully the experimental molecular diffusion.

Aiming improve on computational performance the kinetic model code was submitted to the multi-domain parallel technique with dynamic memory allocation to the loading balance as mentioned in the early section and to the parallel technique utilizing a simple MPI implementation with static memory allocation to the loading balance.

Figure (7) shows the chloride molecular diffusion profile for each code version: serial, parallel and multi-domain parallel for two sub-domains. Where all of them kept the same solution in accordance with the experimental data.

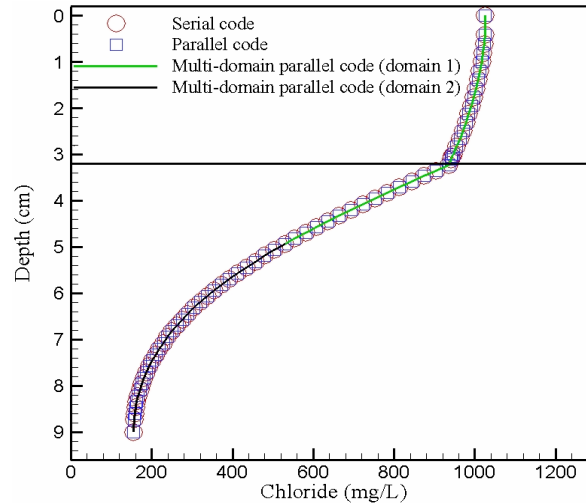


Figure 7. Chloride molecular diffusion profile for each code version

The computational performance of each model version was investigated in order to observe the better strategy. It was carried out limiting the code at 1000 iteration to finish the CPU time measurement. As shown in Fig. (8) the serial code presented a CPU time of 1081 seconds. The simple MPI parallel version running on a cluster of 16 computing node Pentium 4 HT 3.2 GHz with 1 Gb of RAM memory and 1Mb of cache L2 resulted in a CPU time of 128s seconds, where the CPU time dropped until 10 computing node. It occurred due to the network traffic in function of computing node increase. The multi-domain parallel version presented superior performance in comparison with those mentioned previously reaching a CPU time of 84 seconds running on the same cluster machines.

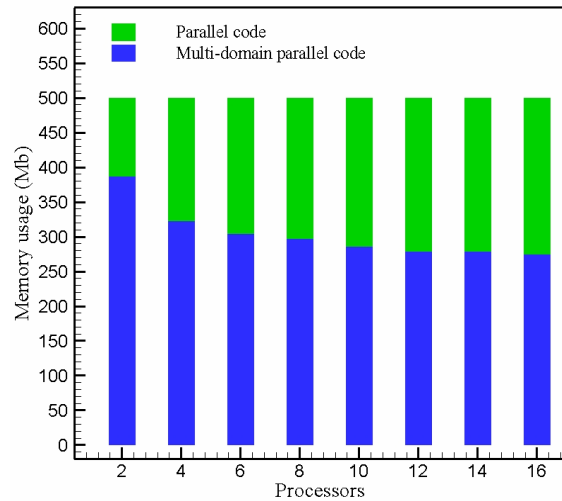
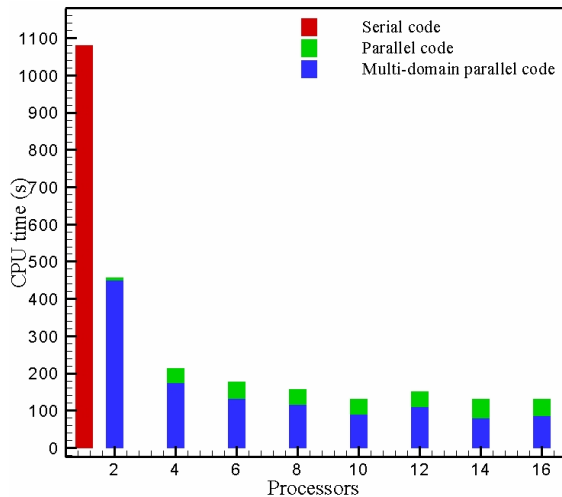


Figure 8. Computational performance of each model version

Figure 9. Memory allocation comparative

As presented in the Fig. (9), the better computational performance of multi-domain parallel in comparison with the simple MPI application can be explained by the dynamic memory allocation efficiency over static memory allocation. This technique provides better RAM and cache memory usage.

As consequence of the computational performance shown above the speedup was calculated and depicted in the Fig. (10). The code speedup can be limited by the higher sub-domain size, therefore, as additional information the estimated speedup in function of the higher sub-domain was calculated and demonstrated join to the linear speedup as well. The Figure (10) shows that the better speedup was reach by multi-domain parallel technique utilizing 14 computing node, resulting in a CPU time 13.85 times faster. However, for the simple MPI application a super linear speedup was noticed until the 8th computing node due to an efficient vector management extracted from the multi-domain parallel technique concept. Where also was observed that the bad loading balance influenced directly the code speedup.

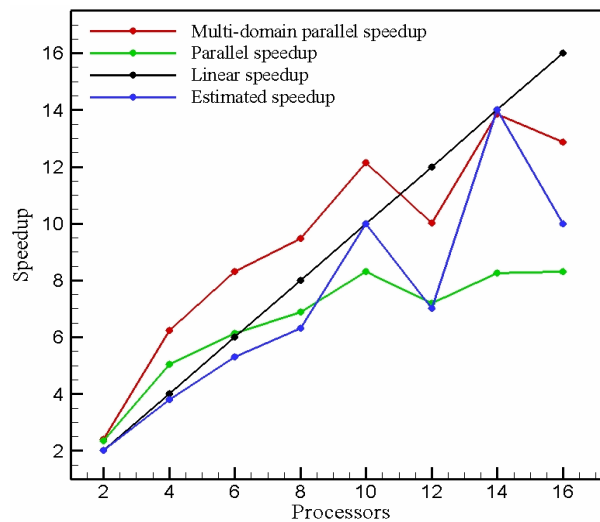


Figure 10. Comparative among each speedup

6. CONCLUSION

In this work a sorption and kinetic mathematical models able to simulate the contaminant transport in the soil was presented. The computational simulation showed the chloride and ammonium molecular diffusion profile for both models. The numerical results was validated through comparison with experimental data where established fine approaching. The results also showed that the inorganic ions migration process can not be explained completely as result of diffusion, but also by the mass transfer phenomenon of contaminant species and the interstitial liquid of the soil to the own soil particle and vice-versa.

Two strategies for the computational code parallelization were presented and in light of computational performance the multi-domain parallel technique proved that can run faster. This work shows that the benefit of dynamic allocation memory is not only for the maximum number of total control volumes that can be linearly increased as the number of computing node was increased, but also it is accompanied by decreasing of CPU time. The loading balance as well as the network traffic was observed as an important performance impact factor where the bad loading balance resulted in a poor speedup.

7. ACKNOWLEDGEMENTS

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