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Reactive Probability of Atomic Oxygen with Material Surfaces in Low Earth Orbit

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A theoretical model based on the theory of molecular dynamics for evaluating the reactive probabilities of the atomic oxygen and highly organized materials in low Earth orbit is proposed. The model is constructed to compute the classical trajectory ensembles by solving a system of stochastic differential equations. The reactive probabilities of the atomic oxygen colliding with atoms on the material surface can then be evaluated in accordance with the criteria proposed for reactive and nonreactive collisions. The computed reactive probabilities for atomic oxygen interacting with graphite are presented as a test case and are compared with flight-test data from STS-46. The model constructed is reliable to some extent as demonstrated in the test case.

Nomenclature

b = impact parameter, Å
D_e^0 = well depth of the Morse potential, eV
D_0^0 = dissociation energy, eV
E_i = initial kinetic energy, eV
$f_{Y_E}(t)$ = random force, N
k_B = Boltzmann constant
M_g = mass of the N_g atoms, kg
M_s = mass of the solid atoms, kg
N_g = labeled gas atoms
N_R = number of the reactive events
N_T = total number of trajectories
P_R = reaction probability
$\langle P_R \rangle$ = average reaction probability
$P_{R\text{-LEO}}$ = reaction probability of the flight experiment
T = surface temperature, K
$V(X, Y_I, Y_E, Y_F)$ = potential energy surface for the full system, eV
X = position of the N_g atoms
Y_E = sets of all edge atoms over all of the layers
Y_F = sets of fixed atoms over all the layers
Y_I = sets of all inner atoms over all of the layers
γ = friction coefficient, Hz
$\delta(t)$ = Dirac function
ε = well depth of the Lennard–Jones potential, eV
ε_{gs} = weighting factor
ε_s = surface effect factor
θ = specific incident angle of the incoming oxygen, deg
θ_D = Debye temperature, K
μ = reduced mass, kg
ξ_{Y_E} = vector of Gaussian random numbers
ω = angular frequency, rad/s
ω_D = Debye frequency, Hz
ω_e = vibrational frequency, cm^{-1}
$\hbar$ = Planck constant

Introduction

THE space environment is characterized by very low pressure, temperature extremes, various atomic or molecular gas species in low concentrations, charged particles, electromagnetic radiation, micrometeoroids, and manufactured debris. All of these species or factors may influence the design of satellites or space stations to a certain extent, depending on the orbital altitude. In the altitude ranges from 200 to 700 km above Earth's surface, one of the primary species present is atomic oxygen at pressures ranging from 10^{-3} to 10^{-5} Pa. Although the atomic oxygen density is only of the order of 10^9 cm^{-3}, because the spacecraft orbital velocity reaches approximately 8 km/s, the actual flux of atoms impinging on an orbiting vehicle is quite high, approximately 10^{14}–10^{15} atoms/cm^2 s. If one takes into account the corotation of the Earth and its atmosphere, the impact energies of the oxygen atoms onto the spacecraft surface can reach 4.4–4.5 ± 1.0 eV. In addition, oxygen atoms are very active oxidizing agents. The energetic collisions between a spacecraft and atomic oxygen in the highly oxidative environment of low Earth orbit (LEO) are favorable for oxidized erosion of material surfaces.

The primary requirements for structural materials used in spacecraft are light weight and high strength. It is for this reason that organic-based materials and carbon-based composites are widely used in spacecraft components instead of metal. Space systems operating in an LEO environment for long periods of time require materials whose properties remain stable within the service lifetime under that environment. Thus, an additional requirement on long service life becomes necessary for the engineering specification of materials used in the spacecraft.

It is well known that oxygen does cause significant erosion to many materials, particularly organic-based materials. At the same time, the high translation energy of the atomic oxygen may also induce physical sputtering on the material surfaces.[1] The reactions of oxygen with a variety of materials was reported by Leger as early as 1982 based on sample loss measurements from the Space Shuttle experiments.[2] Materials such as polymer films and composites are of special interest because of their applications to space structures, space robots, solar arrays, thermal blankets, and second surface mirrors. Experience has shown that even short-term exposure to this environment can have harmful effects on spacecraft surfaces, particularly if they are composed of, or covered with, organic materials. Interactions of energetic oxygen atoms with space materials have profoundly impacted the planning and design of long-duration missions in LEO. As a consequence, the development of a theoretical approach capable of providing reliable data for engineering purpose is essential.

For that purpose, there have been some efforts to develop theoretical models for computing the interaction between atomic oxygen and material surfaces in recent years.[3–6] In the present paper, a theoretical model and the associated numerical procedure based on the classical theory of molecular dynamics are developed. The basic idea of the procedure can be described as follows: The scattering process of an oxygen atom colliding with atoms on highly organized material surfaces is simulated using the procedure of stochastic dynamics. Each computed trajectory from the class of dynamic

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equations is then examined to determine whether or not the associated collision process is reactive. The probability of an ensemble for reactive collisions can, thus, be evaluated accordingly.

Theoretical Approach

The interaction of energetic heavy particles and material surfaces is a highly complex dynamic process. The process is characterized by collision and reaction mechanisms, and with each mechanism, there are various types of physicochemistry effects that can only be treated by different theories. The model presently developed is constructed within the framework of the classical theory of the scattering process. Some simplification is required to make the model workable.

Multizone Model

To model such a process, we start from the theory of molecular dynamics with an assumption that, when the distance of an oxygen atom from the material surface is less than a specified impact parameter, the atomic oxygen will react with the material. Following the idea proposed by Depristo and Metium,[7] we consider a general localized volume region $V_>$ of certain size and shape, in the surface layer of a material. We assume that there are three types of solid atoms in that volume: The first type consists of those contained inside a subvolume $V_<$ that are strongly perturbed by the incoming oxygen atoms. This class of atoms will be treated utilizing the full molecular dynamics and is referred to as the inner atoms. The second type is located on the surface of $V_<$. This group of atoms can be treated by a number of different techniques in the present model and is referred to as the edge atoms. Both of these types of moving atoms can be called active atoms whenever there is no need to distinguish them. The third type of atoms is located outside of $V_<$ but inside of $V_>$ is assumed to be stationary. These fixed atoms are useful in generating a potential with negligible edge effects as a gas atom or solid molecule moves around inside $V_<$. A more important feature for implementing those fixed atoms is their ability to enforce the desired geometry on the moving atoms that are embedded within the fixed atoms.

Let N_g be the labeled gas atoms, and M_g and X be the mass and positions, respectively, of the N_g atoms. Let the positions of the solid atoms be denoted by $Y = (Y_1, Y_2, \ldots, Y_N)$, with N the total number of atoms, and the associated masses be M_s. The local coordinates of the trajectories of the individual components are defined as $X = (x^1, x^2, x^3)$ and $Y_r = (x_r^1, x_r^2, x_r^3), r = 1, 2, \ldots, N$. For computational purposes, we may divide the material in $V_>$ into N_{sl} layers, with the first layer being the surface. For the αth layer, we define two radii, $R_<^\alpha$ and $R_>^\alpha$, with $R_>^\alpha > R_<^\alpha$. The fixed atoms for this layer are those atoms with $(R_<^\alpha)^2 < (x_r^i)^2 < (R_>^\alpha)^2$. The inner and edge atoms satisfy $(x_r^i)^2 < (R_<^\alpha)^2$, with the distinction involving the number of nearest neighbors in the layer: The inner atoms are fully coordinated by other inner and edge atoms in the layer, whereas the edge atoms are not. The sets of all inner, edge, and fixed atoms over all of the layers are denoted by Y_I, Y_E, and Y_F, respectively. The use of different radii for each layer allows for more flexibility in locating the inner, edge, and fixed atoms than simply using the two specified volumes, $V_<$ and $V_>$. In accord with the preceding arguments, the equations for the theoretical model can be constructed as follows.

Dynamic Equations for Gas Particles

All motions of the gas particles follow the classical theory of molecular dynamics, that is, we have

$$M_g \frac{\mathrm{d}^2 X}{\mathrm{d}t^2} = -\nabla_X V(X, Y_I, Y_E, Y_F) \tag{1}$$

where ∇_X is the gradient with respect to the coordinates of X.

It is seen in Eq. (1) that we have made an assumption of neglecting the collision between gas particles because the LEO environment can be considered to be under a free molecular state, that is, independent of gas particle collisions.

Dynamic Equations for Solid Atoms

The dynamic equations for the solid atoms can be constructed in accordance with the aforestated classification of the solid atoms in $V_>$.

Dynamic Equations for Inner Zone

The inner atoms are treated by standard molecular dynamics. The corresponding equations of motion are also given as

$$M_s \frac{\mathrm{d}^2 Y_I}{\mathrm{d}t^2} = -\nabla_{Y_I} V(X, Y_I, Y_E, Y_F) \tag{2}$$

Each atom is assumed to have the same mass M_s for simplicity.

Dynamic Equations for Edge Zone

Random impacts of surrounding particles to the edge particles may, in general, induce two kinds of effects: First, they act as random driving forces on the particle to maintain its incessant irregular motion and can be regarded as the random part of the impact reaction. Second, they give rise to an internal frictional forced motion that can be considered as the systematic part. It is apparent that, because both come from the same origin, the frictional force and the random force must be related. The motion of the edge atoms follow either the theory of classical or Langevin dynamics. Because of the aforementioned reasons, however, a class of Langevin equations involving additional isotropic local frictional and Gaussian white noise type of random forcing terms is adopted. The resulting form gives

$$M_s \frac{\mathrm{d}^2 Y_E}{\mathrm{d}t^2} = -\nabla_{Y_E} V(X, Y_I, Y_E, Y_F) - M_s \gamma \frac{\mathrm{d}Y_E}{\mathrm{d}t} + f_{Y_E}(t) \tag{3a}$$

where

$$\gamma = \pi \omega_D / 6 = \pi k_B \theta_D / 6\hbar \tag{3b}$$

$$f_{Y_E}(t) = (2\gamma k_B T M_s / h)^{\frac{1}{2}} \boldsymbol{\xi}_{Y_E} \tag{3c}$$

Here, h is the time step in the integration and $\boldsymbol{\xi}_{Y_E}$ is the vector of Gaussian random numbers.

We note that Eq. (3b) provides the assurance of a long-time energy transfer into the bulk system if given correctly, whereas Eq. (3c) ensures the correlation of frictional and random forces to obey the second fluctuation–dissipation theorem, that is,

$$\left\langle f_{Y_E}(t) f_{Y_E}(0)^T \right\rangle = 2\delta(t) \gamma M_s k_B T 1 \tag{4}$$

The proof of the second fluctuation–dissipation theorem clearly shows that the correlation between the dissipative and random forces can intimately be related to the requirement that the system relaxes to thermal equilibrium.

Fixed Atomic Zone

The fixed atoms surround the active atoms and are not allowed to move. These stationary atoms provide a structural template for the surface and smooth out the potential energy of the active atoms.

Interaction Potential

The class of Eqs. (1–3) can be solved in a straightforward manner, provided that the interaction potentials for atomic oxygen and solid materials are given. To construct the potential function, all of the atomic structure and the internal interaction potentials of the material, as well as the potential between oxygen and the solid atoms, must be known. It is not possible at the present stage to develop a unified representation of the interaction potential theoretically because of the complexity of the particle systems.

A phenomenological approach to construct a certain potential for a specific material will be illustrated by the atomic oxygen with graphite solid in a later section.

Method of Solution

The classical equations of motion described earlier can be solved by the standard Verlet algorithm.[8] The reaction probability can then be estimated by the trajectories solved for the sample particles.

Numerical Procedure

The initial velocity vector of an oxygen atom can be specified according to the given velocity distribution of the atomic oxygen species over the body under consideration. In the present work, it is assumed to be a given parameter. The positions of the atoms in the material surface are initialized using a Monte Carlo method, and the initial velocities of the surface particles must be specified.

At each integration step, the random forces $f_{Y_E}(t)$ appearing in Eq. (3a) are randomly selected from a Gaussian distribution as given in Eq. (3c). During the computation, a sufficient number of sample trajectories for each incident angle of the oxygen atom must be counted to obtain the required statistical properties.

A trajectory will be terminated when one of the following requirements is met.

1) The distance of an atomic oxygen from the material surface is less than the impact parameter b of the collision process.

2) The number of time steps for the trajectory exceeds a preassigned number of time steps for the numerical integration.

3) The distance between an oxygen atom and the material surface becomes larger than the effective radius of the interaction potential.

4) The oxygen atom is laterally out of the active zone $V_<$ of the material surface, but remains within the interaction range $V_>$ of the surface.

Reaction Probability

Recall that b is the impact parameter for the collision process of the oxygen atoms with the atom on the material surface. An assumption is made that the reaction process of an oxygen atom with an atom in the material surface will have taken place when the distance of the oxygen atom from the material surface is less than b. Accordingly, the reaction probability can, thus, be determined as

$$P_R = \frac{N_R(b;\, E_i;\, \theta)}{N_T(b;\, E_i;\, \theta)} \tag{5}$$

where the number of reactive events N_R and the total number of trajectories N_T are both functions of b as well as the initial kinetic energy E_i and the specific incident angle of the incoming oxygen θ.

Reactive Interaction Between Atomic Oxygen and Graphite Surface

Numerical results for the reactive interaction between an atomic oxygen and a graphite solid are presented as an illustration.

Reaction Potentials for Interaction Between Atomic Oxygen and Graphite Surface

In the present calculations, the graphite lattice is assumed to be perfect and hexagonally close packed as shown in Fig. 1. The layers of solid graphite are ordered according to ABAB . . . stacking with lattice constants $a = 2.46$ Å and $c = 6.70$ Å. The Debye temperature for graphite is readily evaluated to be $\theta_D = 420$ K (Ref. 9). The interaction potentials for the particle system can be obtained as follows.

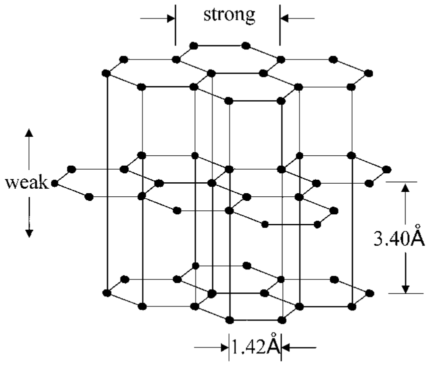

Fig. 1 Close-packed lattice structure of graphite, ABAB ▷▷▷stacking.

Potentials for Carbon–Carbon Atoms

We assume that all of the potentials between carbon atoms are induced by the harmonic oscillators. The Lennard–Jones potential is, thus, adopted, that is,

$$V(r) = 4\varepsilon\left[(r_e/r)^{12} - (r_e/r)^{6}\right] \tag{6}$$

The potential parameters ε and r_e are readily obtained as 45.16 meV and 3.35 Å, respectively.

Interaction Potentials Between Atomic Oxygen and Carbon Atoms

The theoretical descriptions of the interaction between incoming particles with a surface are highly dependent on the energy with which the interaction takes place. The mass of the projectile and the corresponding momentum transfer to the solid are also important factors for the choice of a theoretical description of the interaction. As pointed out by Tenner et al.,[10] from low (thermal) to high (10 keV) energy, the surface may be viewed as evolving from a flat hard wall, through first a corrugated hard, then corrugated soft, surface to an arrangement of individual atoms. Consequently, theories have to treat the surface, correspondingly, as a homogeneous electron density, a hard flat or corrugated wall, a set of soft cubes, or as individual atoms in a lattice. Each description has some validity for a specific energy range. However, in some intermediate regions, some mixed descriptions may occur. In these energy regions, the particle–surface interaction may not necessarily be described as a series of purely binary interactions of the incoming particle with the surface atoms, nor can it be expressed in terms of a corrugated surface potential. For this reason, we assume that the incoming atomic oxygen will interact with a number of target atoms on the material surface simultaneously. We may, thus, introduce a surface effect factor ε_s into a classical potential function to account for the effects induced by a few surface atoms on the projectile particle.

On the other hand, for higher collision energies, where the structure regime applies, the gas atoms experience a rougher potential dominated by the repulsive interaction with individual surface atoms; the predominant part of the potential is repulsive.[10,11] Hence, the attractive part of the potential is not important for the present test case. It is for this reason that we multiply the attractive part of the potential by a weighting factor ε_{gs} to reduce the influence of the attractive potential.

For the interaction potential between an oxygen atom and the graphite surface, it is more reasonable to use the Morse potential, and the Morse potential for carbon monoxide appears to be the most convenient choice for presenting the interaction potential between an oxygen atom and the graphite surface. Accordingly, we adopt the following interaction potential:

$$V(r) = \varepsilon_s D_e^0\{\exp[(r_e - r)/a] - 2\varepsilon_{gs}\exp[(r_e - r)/2a]\} \tag{7}$$

where D_e^0 is the depth of the potential well given as

$$D_e^0 = D_0^0 + \hbar\omega/2 = D_0^0 + hc\omega_e/2$$

$$a = \omega\left(\mu / 2D_e^0\right)^{\frac{1}{2}} = 2\pi c\omega_e\left(\mu / 2D_e^0\right)^{\frac{1}{2}}$$

and r_e is the equilibrium interaction distance or the collision diameter, h Planck constant, and c the speed of light in vacuum.

By virtue of the available data of molecular properties for carbon monoxide,[12] we obtain $D_e^0 = 11.23$ eV and $a = 2.33$ Å^{-1}. In principle, the surface factors ε_s and ε_{gs} will be determined empirically. For our simulation, they are chosen to be $\varepsilon_s = 14.0$ and $\varepsilon_{gs} = 0.3$, respectively.

Given Conditions for Numerical Test Case

To provide initial conditions for the velocity distribution in the material surface, before any calculations of the atom–surface interaction are performed, a few layers of graphite under thermal equilibrium at $T = 394$ K must be obtained.

The system considered in the present computations consists of an oxygen atom and six layers of carbon atoms. The initial translation energy of an oxygen atom is set at 5 eV. Then the initial velocity vector of an oxygen atom can be determined from the initial translation kinetic energy. The polar angle from the surface normal, θ, is equal to the incident angle for each case, and the azimuthal angle from the x axis $\phi = 0$. The specified value of the initial height above the surface is 12 Å, whereas the initial position is randomly sampled over the substrate unit cell.

The Miller index of the graphite surface is (100). All calculations have used 105 inner atoms, 228 edge atoms, and 2117 fixed atoms. The positions of the surface atoms are initialized using a Monte Carlo method. The initial velocities of the surface are sampled from a Maxwell–Boltzmann distribution for $T = 394$ K.

The time step for integrating the equations of motion is set to be 0.2 fs. At each integration step, the random forces $f_{Y_E}(t)$ are randomly selected from a Gaussian distribution for Eq. (3c). For each incident angle we calculated 1000 trajectories to obtain the required statistical properties. Because the parameter r_e in Eq. (7) can be regarded as the impact diameter of the atomic oxygen with the graphite surface, we may assume that the impact parameter $b = r_e/2$.

Numerical Results

The reactive probabilities for various incident angles and the average reactive probability for given ε_s and ε_{gs} are summarized in Table 1, together with the data collected for an atomic oxygen etching over the graphite during the STS-46 mission.[13] Because the latent heat of graphite, that is, the threshold energy for sputtering, is 170.9 kcal/mol = 7.41 eV, it is far in excess of the average oxygen incident energy for an orbiting spacecraft. Furthermore, even if the translation energy of the oxygen atom were as high as 6.5 eV, it would be unlikely that a sufficiently large surge of vibration energy from the solid would lead to ejection of a carbon atom. Hence, the atomic oxygen etching of graphite in LEO, that is, one C atom for every eight incident O atoms, is regarded as the reactive probability of the graphite, $P_{R\text{-LEO}}$. By comparing the average reactive probability computed by the present theory, $\langle P_R \rangle$, with $P_{R\text{-LEO}}$ obtained by flight mission, there is 34% deviation.

The reactive probability dependence of the incident angle is shown in Fig. 2. As can be seen, the tendency of the reactive probabilities to vary with the incident angles is similar to the numerical results of the reactive probabilities computed for atomic oxygen with adsorbed carbon monoxide on a platinum surface as given by Ree et al.[14] As the incident angle increases, the interaction between the incident oxygen atom and the carbon atom of the graphite surface weakens, leading to less efficiency in energy transfer from the incident oxygen atom to the carbon atom of the graphite surface.

Table 1 Reactive probability for ε_s = 14 and ε_{gs} = 0.3[a]

θ, deg	P_R
0	0.231
10	0.246
20	0.217
30	0.196
40	0.167
50	0.140
60	0.135
70	0.156
80	0.028

[a] Average probability overall P_R, that is, $\langle P_R \rangle = \Sigma P_R/9 = 0.168$. Mission-obtained probability $P_{R\text{-LEO}} = 0.125$.

Table 2 Reactive probability for ε_s = 4.0 and ε_{gs} = 0.4[a]

θ, deg	P_R
0	0.446
10	0.472
20	0.428
30	0.352
40	0.327
50	0.279
60	0.245
70	0.233
80	0.089

[a] Average probability overall P_R, that is, $\langle P_R \rangle = \Sigma P_R/9 = 0.319$. Mission-obtained probability $P_{R\text{-LEO}} = 0.125$.

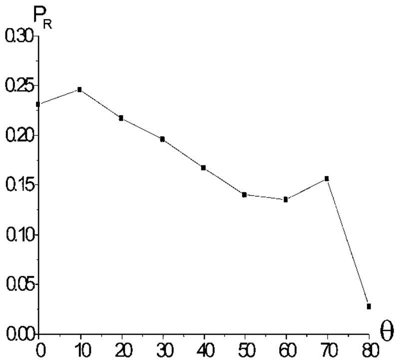

Fig. 2 Incident angle dependence of reaction probability for ε_s = 14 and ε_{gs} = 0.3.

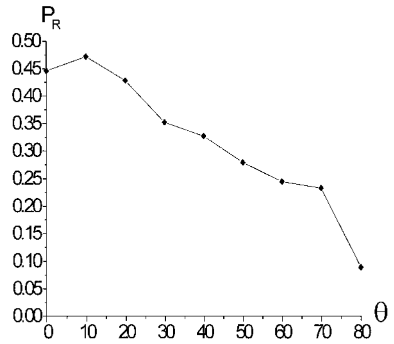

Fig. 3 Incident angle dependence of reaction probability for ε_s = 4.0 and ε_{gs} = 0.4.

Based on the in-space generally accepted erosion yield for pyrolytic graphite of 1.2×10^{-24} cm^3/atom and a density of 2.2 gm/cm^3, if one assumes carbon is oxidized through the formation of carbon monoxide, then a reaction probability of 0.13 is produced. This is based on measurements with atomic oxygen arriving at normal incidence. As shown in Fig. 2, however, the probability at normal incidence obtained by the present model is 0.231, significantly higher than the just stated value. One of the reasons for the deviation is the lack of reliable data to correlate the surface factors ε_s and ε_{gs}. To verify the uncertainties of the values of the surface factors, we conducted a series of numerical experiments with different surface factors ε_s and ε_{gs}. The numerical results reveal that the reactive interaction between atomic oxygen and graphite surface drops as ε_s increases or ε_{gs} decreases, because the repulsive force between oxygen and carbon atoms tends to increase under these circumstances. Table 2 and Fig. 3 give the related results at various incident angles for the case of $\varepsilon_s = 4.0$ and $\varepsilon_{gs} = 0.4$ and the associated average reactive probability. It is seen that the deviation from $P_{R\text{-LEO}}$ is larger than the preceding test case.

Because the space environment is highly complicated, the reactive probabilities correlated from distinct flight conditions under different flight missions differ significantly from each other. For vitreous carbon and graphite, some of the data differ by nearly one order of magnitude; compare, for example, Refs. 15 and 16. These references pointed out that the results of the flight experiments are also very different from those of the ground simulations even though the same materials are used, for example, graphite. In light of this, the results obtained by the present model are acceptable.

Conclusions

A theoretical model for predicting the reactive probability of translationally energetic oxygen atoms with material surfaces of highly organized structures was developed. The interaction of atomic oxygen with graphite was then computed utilizing the model and compared with the flight data.

The numerical experiments performed in the present work demonstrated that the construction of validated interactive potentials for atomic oxygen vs various materials is the crucial part of the theory. Because of the scattering of the data collected from flight tests, it is not possible at the present stage to correlate the surface factors ε_s and ε_{gs} reliably with the available data. Further theoretical work must be pursued to resolve the problem. Nevertheless, the theory of stochastic dynamics presently developed has demonstrated the feasibility for the model to provide an avenue for exploring the interactive mechanisms between space particles and surface materials in orbital environments.

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