**Types of collisions**

There are seven possible collisions between plasma and background gas species for a single metal oxide target with formula . For an oxide target with two metals and general formula there are twelve possible collisions: (1-3) for collisions between either one of the atoms in the plume and stationary background particles, (4-6) for the collisions of the plume atoms with high energy propagating background particles, (7) , (8) , (9) , for two identical particles within the plasma, (10) for collisions between the two metal atoms, and finally (11, 12) for collisions between the metal atoms and the oxygen atoms originating from the target. As result of an inelastic collision an oxidation reaction can occur, introducing new plume species with formulas , which increases the number of collision terms.

The initial velocity distribution separates identical particles in space, which means collisions between identical particles are relatively rare. When two identical particles with different velocities, traveling in the same direction, collide elastically, their velocities interchange. This results in a zero-net change in the plasma particle velocity distribution. Therefore, identical particle collisions are neglected.

If the two metal atoms are of similar mass (e.g. ), their initial average velocities will be close to each other. In this case the cross term is expected to be large. If the masses of the two metals vary greatly (e.g. ), their initial average velocities will be spaced apart, and consequently they will separate in space, resulting in a small collision term. However, if a significant amount of light metal atoms gets slowed down by the background gas, the heavy metal atom might still collide with the light metal, which would again increase the significance of the collision term.

**Collision probability**

* *Generalize for collisions with either background gas or other plasma species (plasma particle and collision medium)*

The paper by Wijnand considered the collision probability of a plasma particle colliding with a background gas particle to be:

Wijnand’s proposed collision probability within time interval is a function of the plasma particle velocity , and the background gas particle velocity . It is determined by the velocity of the plasma plume , the scattering cross-section , and the local density of particles of the background gas , with for the current radial bin, for the current angular bin, for the velocity bin of the background gas particle, and for the current time step. The scattering cross-section is determined as the sum of the cross-section of two colliding hard spheres with atomic radii. In the case of molecules, the hard sphere radius is assumed to be the sum of the atomic radii of its components, so in the case of O2 the cross-section will be , where is the atomic radius of oxygen. The local particle density of the background gas must be determined per velocity bin. As all background particles are initially assumed to be static, they all start out in the first velocity bin . Note that this expression is not a normalized probability, the factor gives the volume of the path traversed by a particle within one timestep, multiplying this by the density gives the number of particles within this volume. If the number of particles in this volume is greater than one, the collision probability is effectively 100%, as it is guaranteed there is at least one particle within its path.

There are some problems with this approach. Due to the high velocities of the plasma, multiple radial bins can be traversed within one time step, this makes it unclear which particle density to use in the expression. Also, the expression does not account for the relative difference in velocities between the plasma particle and the background particle. Logically, a plasma particle will never collide with a particle with the same or higher velocities, so if then . Also, one would assume there is a higher probability of colliding with a background particle with a lower relative velocity. It is important to include this if we want to accurately model collisions between different plasma species with similar velocities. A practical problem with calculating the number of particles that get scattered is the conservation of number of particles, as it must be ensured that no particles are destroyed or created.

To address these issues, a new approach was developed. In Wijnand’s model, all particles that collide are assumed to collide based on the background particle density in the radial bin where the particle left off. If a particle traverses multiple radial bins within one time step, it is impossible to know in which radial bin the particles scattered. It is important to know this in order to accurately update the number of plasma and background particles in each bin per time step. There are two approaches to this. The first one is two calculate the collision probability for each traversed radial bin, based on the local background particle density, where only the fraction of particles that did not collide can traverse to the next radial bin. The second approach is to calculate the collision probability for the entire traversed path based on the average density and assume there is an equal probability of scattering within each bin. The first approach arguably closer resembles reality, although it increases the computational cost as one must include at least one additional loop over the traversed path. However, the use of the second approach can be justified by the quantized nature of the model, as one does not have any knowledge as to what happened between each time step, so assuming an equal fraction of collided particles gets scattered in each traversed bin is a fair assumption. A problem with the second approach is that if you do not know with which velocity and in which radial bin a collision happens then you cannot accurately update the number of particles. How we tackle this problem is with the assumption that a plasma particle will collide with the lowest velocities first. Only when all the particles in the lowest velocity bin have been scattered, the plasma particle will collide with the background particles within the next lowest velocity bin.

Let us continue with the second approach which will be formulated mathematically. The number of radial bins traversed by a particle moving with velocity within one time step is given by:

The average density of these traversed bins is:

The collisions probability is written slightly different:

Which we extend with a factor that accounts for the relative difference between the plasma and background particle velocities:

So, now if no collision takes place, and collision is more likely between particles with a higher difference in velocity.