

PARTICLES ANALYZER

The module is used to analyze properties of particles and export data as file in text format. Data for the analysis is taken from the results file (*.mdem), therefore saving step which was used during the simulation can influence the accuracy of the results. Linear interpolation is used to obtain data between saved time points.

User can obtain information about the following parameters of particles (*Fig. 1 - Property*):

- *Coordinate*: distribution of particles according to space coordinates;
- *Coordination number*: distribution of particles according to coordination number;
- *Distance*: distribution of particles according to the distance to specified point or line. It is possible to specify point or line to which the distance should be calculated;
- *Force total*: distribution of particles according to the total force acting on them;
- *Kinetic energy*: distribution of particles according to kinetic energy;
- *Max overlap*: distribution according to overlap between particles. For each particle only one overlap with the maximum value is taken into account.
- *Number*: total number of particles;
- *Potential energy*: distribution of particles according to potential energy. Is calculated related to the origin of coordinates.
- *Residence time*: residence time of particles in given volumes (more detailed description below);
- *Total volume*: total volume of particles;
- *Velocity total*: distribution of particles according to velocity;
- *Velocity rotational*: distribution of particles according to rotation velocity.

Four following results types can be selected (*Fig. 1 – Results type*):

- *Distribution*: distribution of selected parameter by specified number of classes on specific time interval (list of time points, see below). In this case the results will be generated as a table where each row represents a time point and each column corresponds to the specified property interval. Each cell of the table contains number of particles which have property value within the given interval;
- *Average*: the result is an arithmetic average value of selected property for each time point. Additionally the information about number of considered particles and deviation for each time point will be provided in results;
- *Maximum*: maximum value of selected property for each time point;
- *Minimum*: minimum value of selected property for each time point.

For such properties as *Coordinate*, *Distance* to point, *Total Force*, *Total* and *Rotational Velocity* besides the magnitude (*Length*) a specific component of resulting vector (*X*, *Y*, *Z*) can be determined (Fig. 1 – *Vector component*).

Each property can be obtained for specific time interval, divided into classes (Fig. 1 - *Time*). Values will be exported for each time point from interval $[T_{FROM}; T_{TO}]$ starting from T_{FROM} with specified time step ΔT . For example for initial data $T_{FROM} = 0$ s, $T_{TO} = 5$ s, $\Delta T = 1$, the results will be generated for time points 0, 1, 2, 3, 4, 5 s. To get values for only one specific time point T specify $T_{FROM} = T_{TO} = T$. There is also a possibility to obtain results only for those time points, which were saved during the simulation (thereby avoiding the interpolated results).

To analyze distribution of some property (*Results type: Distribution* is chosen), there is a possibility to specify range of values for selected property and number of classes on which this interval will be divided (Fig. 1). Particles whose properties do not fall within a predetermined range **will not be considered**. The result for each class at a specific time point is a number of particles whose properties fall within this class. If the value is exactly on the boundary between intervals, it will be assigned to a greater interval.

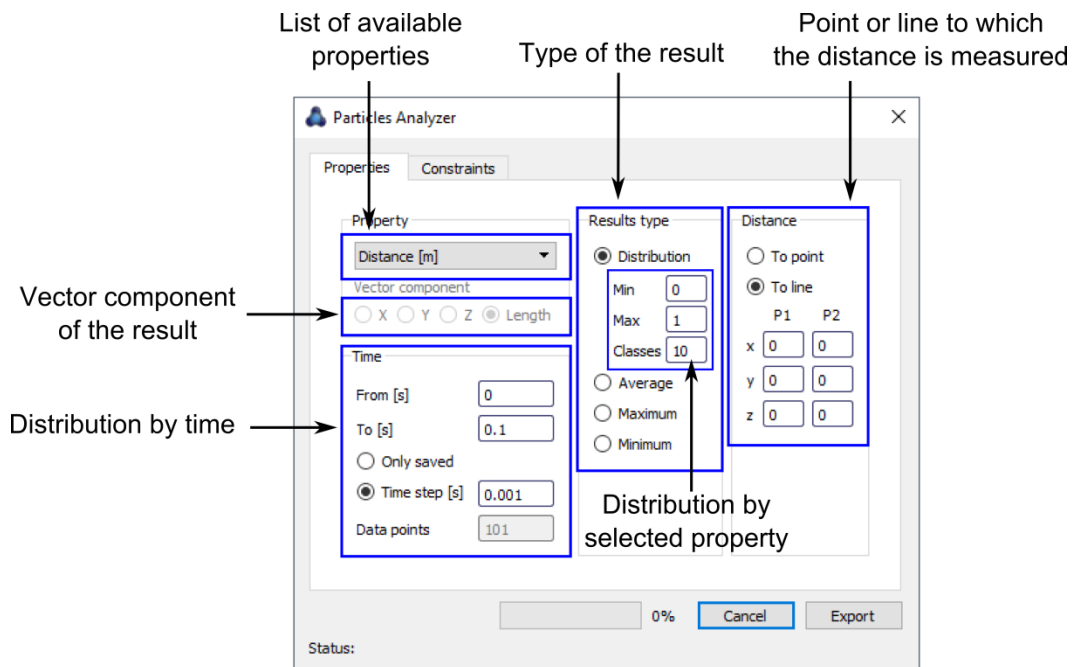


Figure 1. Main dialog of the Particles Analyzer.

In the case of *Residence Time* analysis, T_{FROM} and T_{TO} define the time interval which will be used for analysis. This time interval is afterwards divided into classes and positions of particles at each time step is analyzed. If center of particle at time point T_i was not situated in the analysis volume and at the next time point T_{i+1} it was, then T_i is considered as time of border intersection (Fig. 2). Similarly, T_j will be considered as time when particle leaves analysis volume. The residence of particle will be calculated as

$T_j - T_i$. Therefore, number of data points has influence on accuracy and should be set high enough to avoid analysis error.

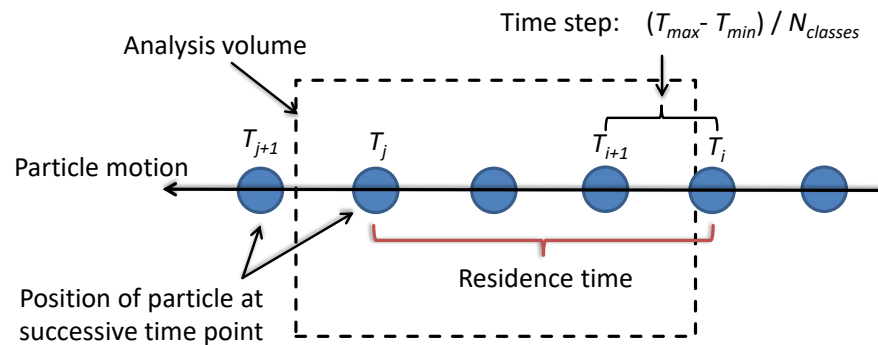


Figure 2. Calculation of residence time.

One or several constraints can be applied in Particles Analyzer (Fig. 2) (turning on filters can slightly reduce performance of the analysis):

- **Materials:** only particles of selected materials will be taken into account;
- **Volumes:** only particles which are within one of selected analysis volumes will be taken into account;
- **Diameters:** only particles with diameters within specified interval will be considered.

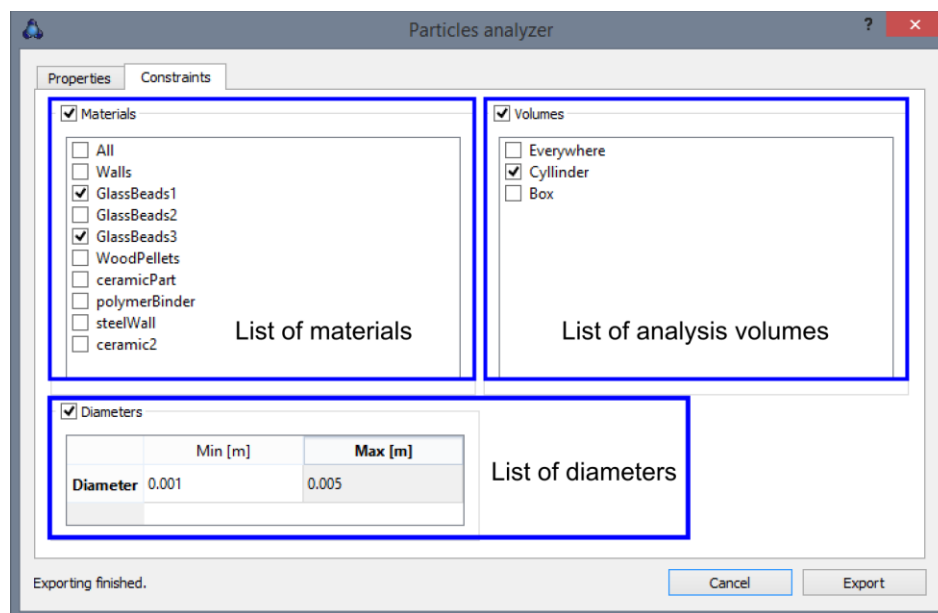


Figure 3. Constraints specification for Particles Analyzer.