

# PARGAN: an inverse modeling procedure to investigate empirical aerosol population dynamics in smog chambers

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Within this project the inverse model PARGAN (particle growth and nucleation) has been further improved, tested, and used. A user interface has been created to enable easier use of the program.

A detailed description of the model has been described in the literature<sup>1</sup>. It is based on a regression analysis of the General Dynamic Equation (GDE) to fit the measured change of the aerosol size distributions in time, which are used as input for the model. This leads to a best-fit estimate of e.g. the particle wall loss rate or the particle growth rate. Based on a time series of the growth rate, the time of nucleation of measured particles of a certain size can be determined. The nucleation rate is then obtained by integrating the particle losses from time of measurement to time of nucleation.

The program includes a full description of aerosol population dynamics (condensation, coagulation, deposition), of which several factors can act as fit parameters, and its potential use is therefore broader than the determination of nucleation and growth rates. Empirical rates of deposition, mixing, or coagulation can also be determined.

The growth rate obtained via PARGAN is more sensitive than the common method of fitting a curve through the banana-shaped contour plot of consecutive size distributions or taking the time derivative of the modal (or mean) diameter. This can be a benefit, e.g. by obtaining more detailed information on the time evolution of the growth rate, but it can also be a drawback if some of this information is due to spurious measurement variability. Several means of error analysis have been investigated in an attempt to minimize the sensitivity to spurious changes in the measured size distributions.

Some results of applying PARGAN to smog chamber measurements of isoprene oxidation at PSI will be shown. PARGAN is also used by Professor Shanhu Lee's group of Kent State University and by Mike Mozurkewich's group at York University.

A user interface has been written in PHP by Dr. Jörg Mäder and hosted by the ETH Zurich on <http://iacweb.ethz.ch/php/pargan/index.php>. The user interface and the adapted IGOR program, which is being called from the php-script, run on a network-based virtual PC. The user needs to provide several input data (measurements and environmental parameters). It offers less flexibility than running the program directly from IGOR, but the advantage is that no knowledge of the program is needed.