

# Scientific report for ESF grant 5297

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## 1. Purpose of the visit

The purpose of the visit was to combine the knowledge of modeling of streamer discharges from the group from CWI, Amsterdam with the knowledge of plasma chemistry from the group of Dr. Francisco J. Gordillo Vázquez, Granada, Spain.

## 2. Description of the work carried out during the visit

During visit Dr. J. Gordillo Vázquez, Dr. A. Luque and I specified exact topic “determining of all significant pathways in chemical reaction systems”. After long discussions we come up with an algorithm and I started a practical implementation of it. The work is still in progress. The motivation was the following: when the output of a complex chemical model is analysed, a typical topic is the determination of pathways, i.e., reaction sequences, that produce or destroy a chemical species of interest. A representative example is the investigation of catalytic ozone destruction cycles in the stratosphere. An algorithm for the automatic determination of pathways in any given reaction system is specified. Under the assumption that reaction rates are known, it finds all significant pathways, i.e., all pathways with a rate above a prescribed threshold. The algorithm forms pathways step by step, starting from single reactions. The chemical species in the system are consecutively considered as ‘branching points’. For every branching-point species, each pathway producing it is connected with each pathway consuming it. Rates proportional to ‘branching probabilities’ are calculated. Pathways with a rate that is smaller than a prescribed threshold are discarded. If a newly formed pathway contains sub-pathways, e.g., null cycles, it is split into these simpler pathways.

## 3. Description of the main results obtained

We obtained quite preliminary results indicating that algorithm is working. The major part of the software program is done.

## 4. Future collaboration with host institution

We are in active collaboration now. In future we plan one more visit to host institution in order to discuss the results and future publications.

## 5. Projected publications / articles resulting or to result from the grant

As mentioned in the sections 3 and 4, the results are preliminary and should be polished further.