Modelling the Formation and Size-Spectrum Evolution of Urban PM with Fast Algorithms

2-Part Presentation

a) Problem Formulation

b) Testing

Goals Aimed

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- For evaluating the importance of aero-disperse particles in atmospheric processes the respective aerosol conservation equations need to taken into account.
- This means several (~70) additional differential equations.
- It is likely that these simulations are prohibitive in CPU times.
- FIA^{2}PES^2 is an <u>implicit</u> numerical algorithm which resolves these problem works with very large time steps while maintaining physical reality.
- It is a vehicle on which well known atmospheric models for nucleation, condensation, deposition etc., could be incorporated and tested.

Structure of the FIA²PES² module

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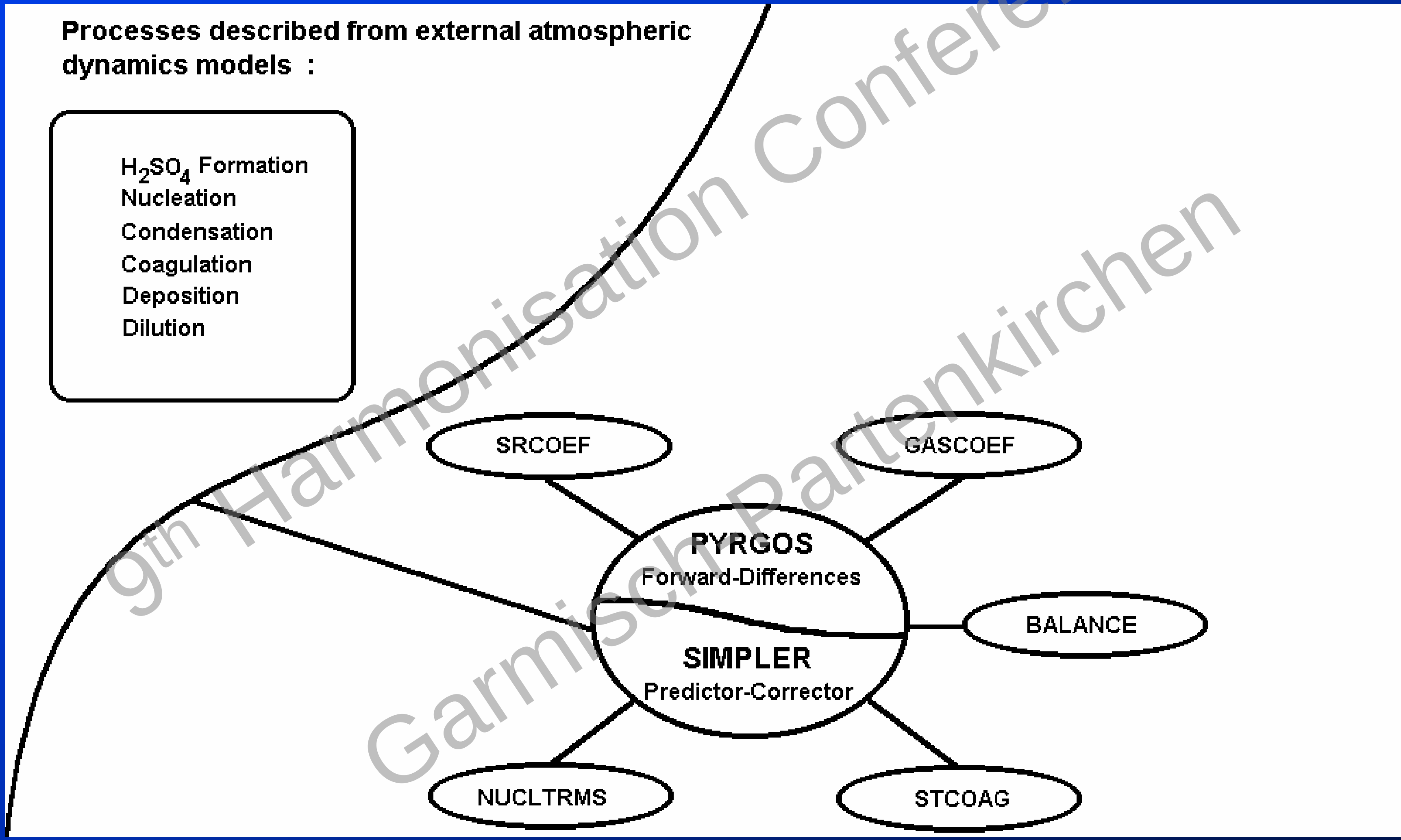

The Particle Size Conservation Eqns

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$$\frac{dS_g}{dt} = R - J\,n_\kappa - \sum_{i=1}^{L} C_i N_i - \lambda_g^{dep} S_g - \lambda_g^{dil} S_g$$

Gas phase equation

$$n_i \frac{dN_i}{dt} = \sum_{j=1}^{L_{i,j}} (n_{j1} + n_{j2}) K_{j1,j2} N_{j1} N_{j2} - n_i N_i \sum_{l=1}^{L} K_{i,l} N_l (1+\delta_{i,l}) +$$

$$+ \frac{n_i}{n_i - n_{i-1}} C_{i-1} N_{i-1} - \frac{n_i}{n_{i+1} - n_i} C_i N_i - n_i N_i \lambda_i^{dep} - n_i N_i \lambda_i^{dil}$$

Particle equation size i

The capabilities of FIA^2PES^2

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- **Variable Nucleation process**
- **Classes with variable width of the size spectrum**
- **De-coupling of coagulation from other processes (possibility to calculate under smaller or larger time steps)**
- **Forward differencing or Predictor-corrector schemes**
- **Implicit/Explicit solutions with <u>inherently</u> positive particle concentrations**
- **Restarting features with realistic initial concentrations**
- **Constant or variable time steps**

Nucleation rate

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New particle formation by nucleation through theoretical expressions for the rate of nucleation, expressed as the number of particles formed per unit volume per unit time.

The approach of M Kulmala et. al. (1998) is used "Parameterizations for sulphuric acid-water nucleation rates, J. of Geophysical Research D 103, pp 8301-8307".

This calculates the nucleation rate and the balance term for the H2SO4 concentration using a revised version of the classic sulphuric acid - water nucleation model.

All of the nucleated particles are transferred to the smallest aerosol size section.

Input conditions

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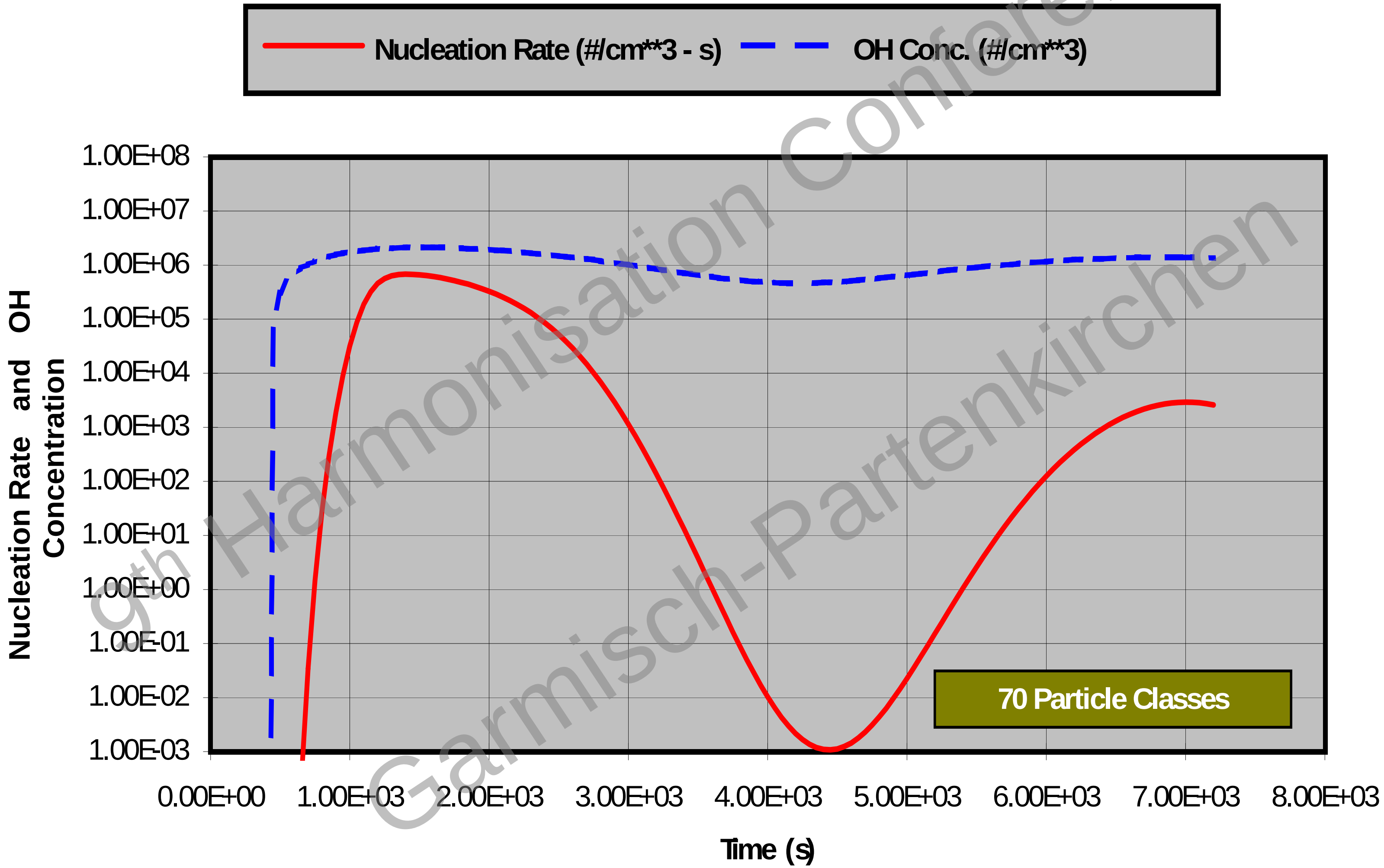

Calculated concentrations

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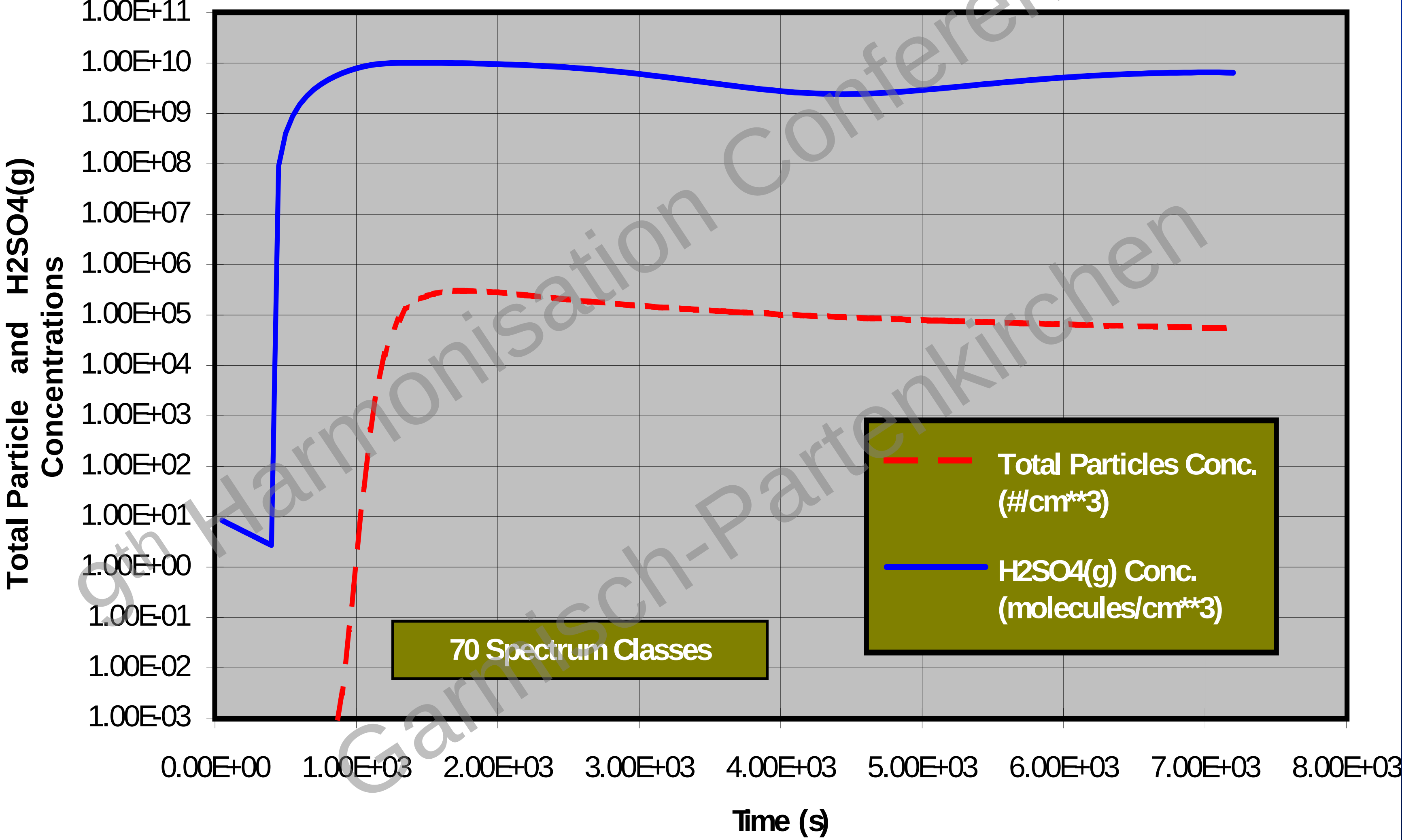

Time evolutions of the Size Spectrum

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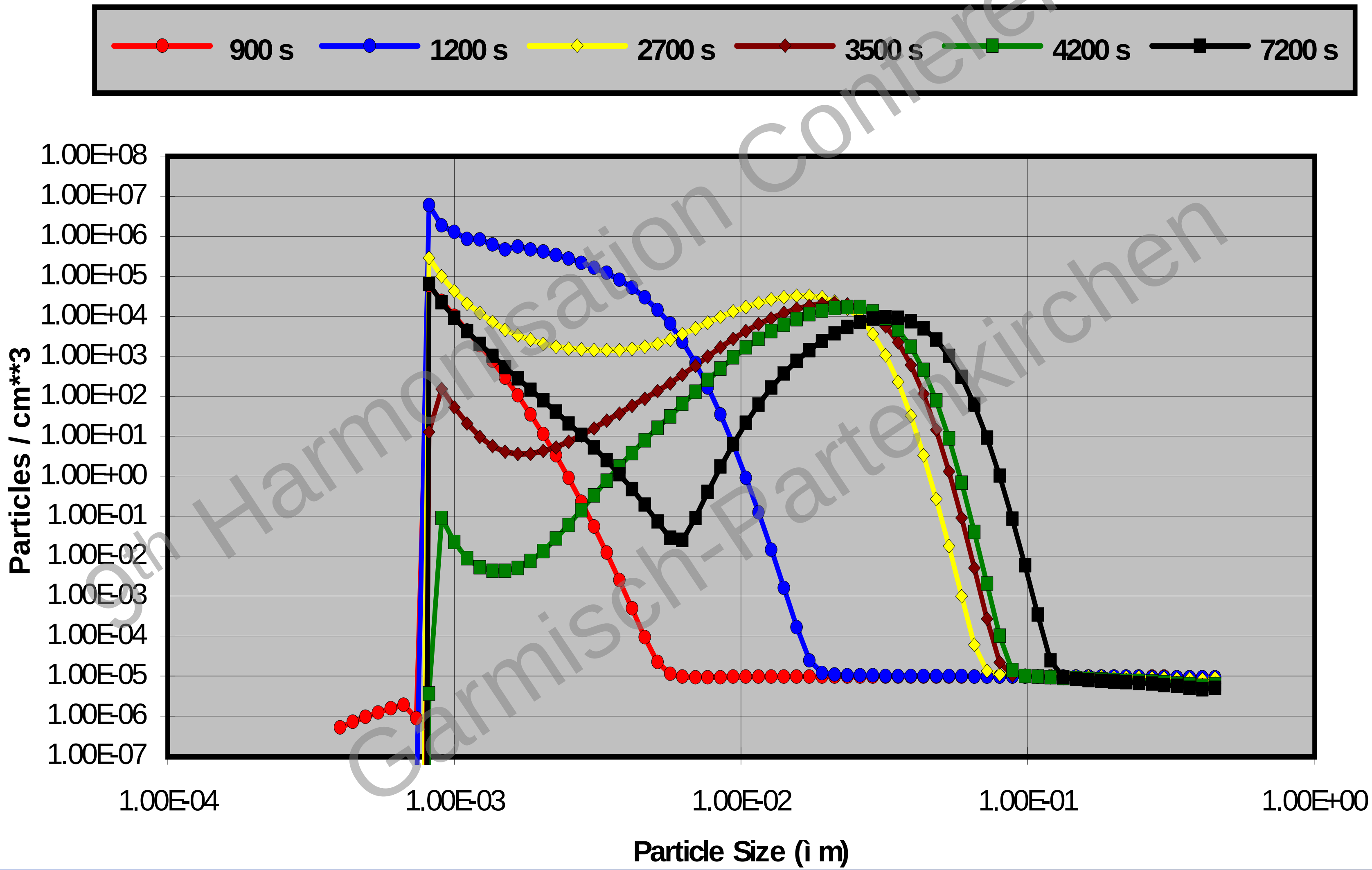

Dependence on the Number of Spectrum Classes (final spectrum distribution)

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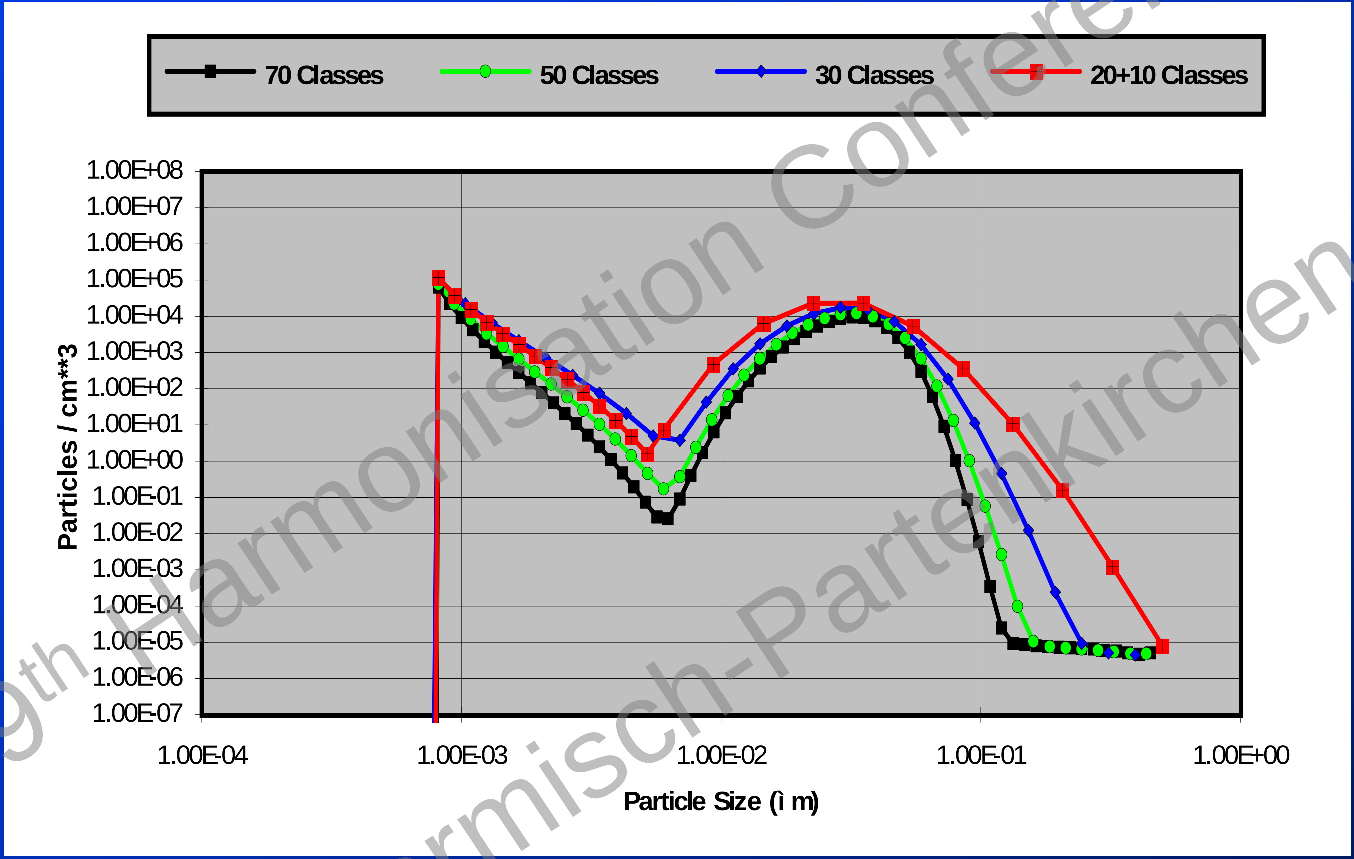

More classes are needed for the small particles

Dependence on the Number of Spectrum Classes (evolution of the concentration)

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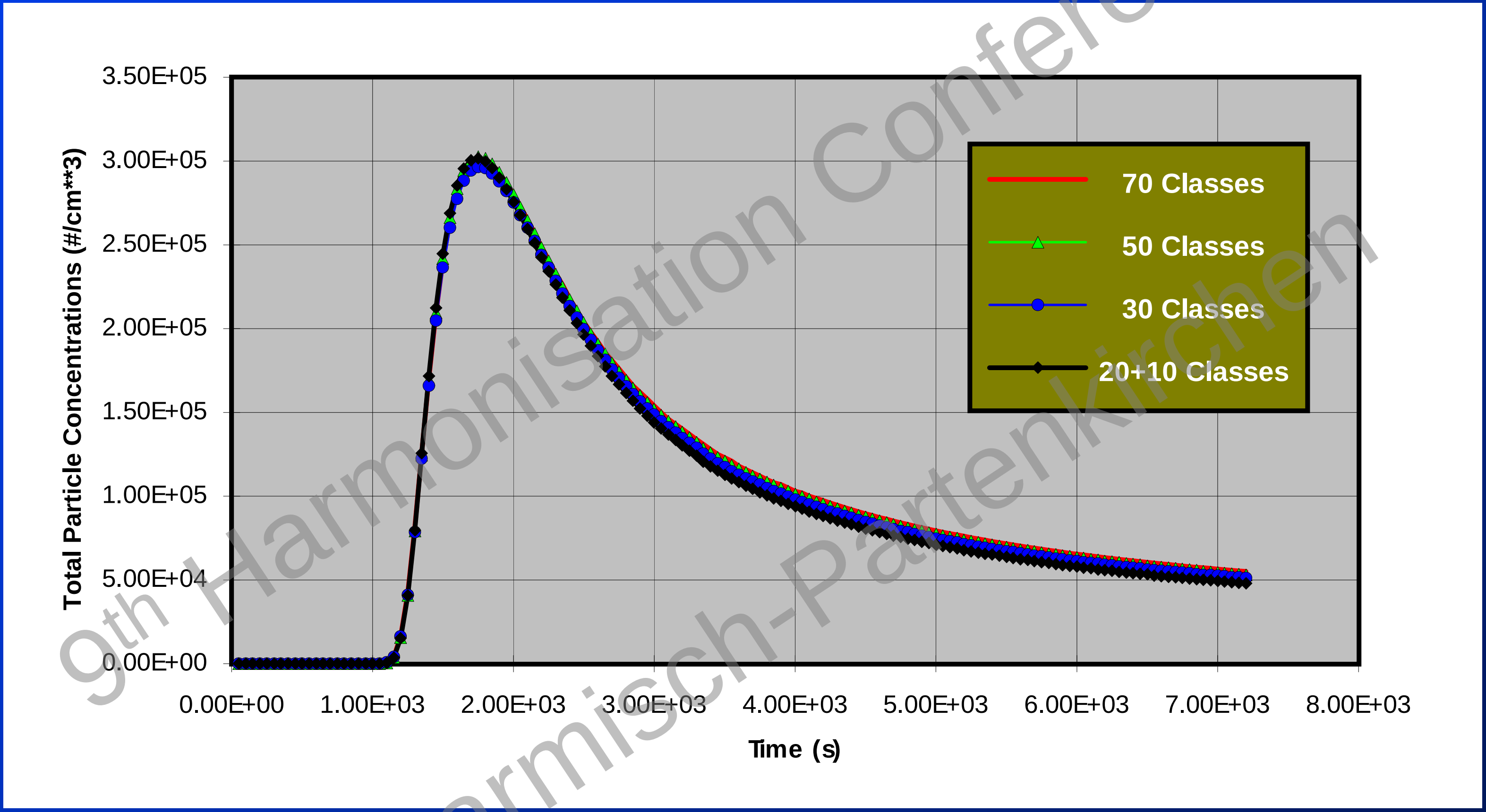

There is no significance differences due to the reduction of the spectrum classes

The Validation of Large Time Steps (final spectrum distribution)

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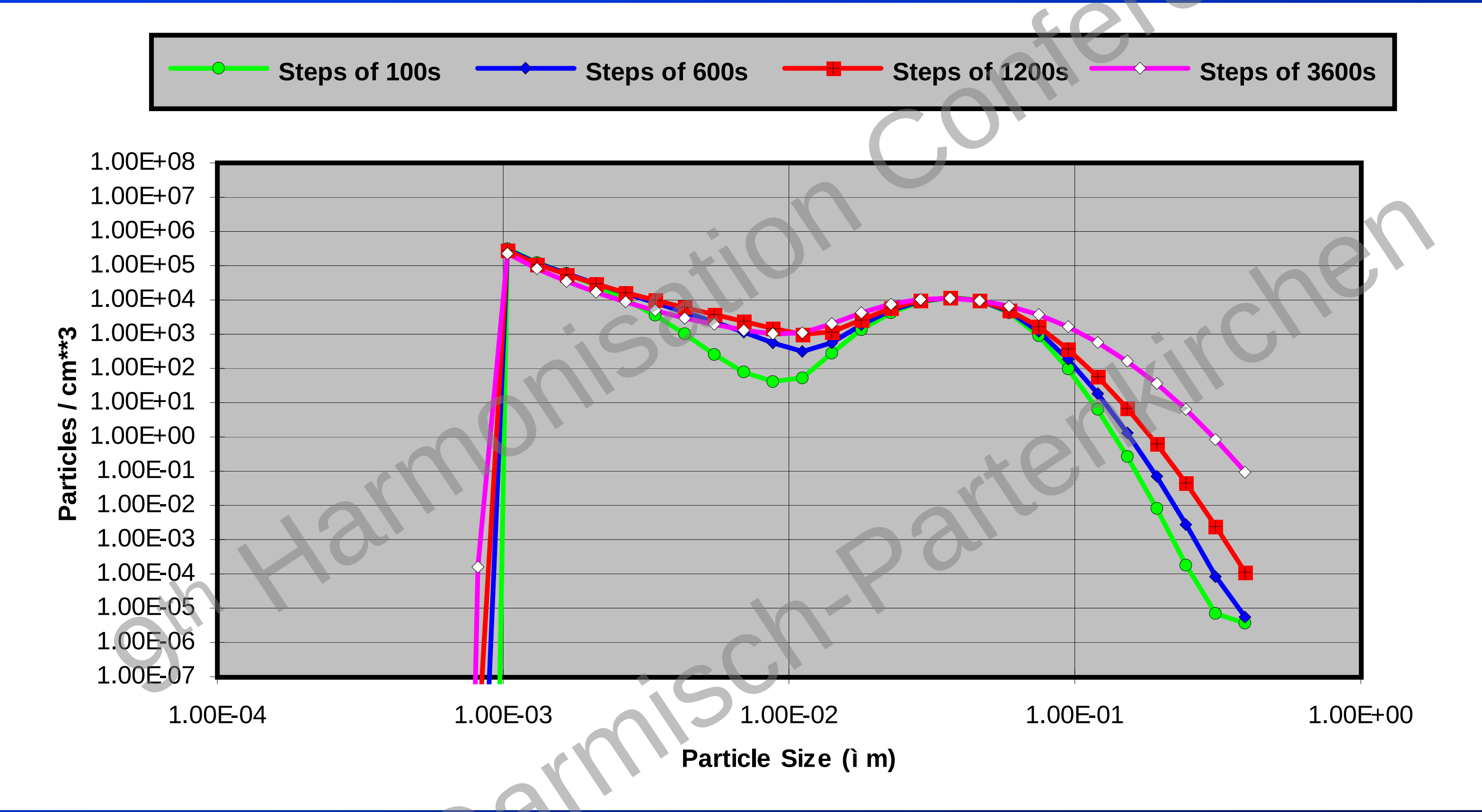

A 2h simulation carried out with constant nucleation rate in a close container As initial particle concentrations was taken the values at 1h.

The Validation of Large Time Steps (evolution of the concentration)

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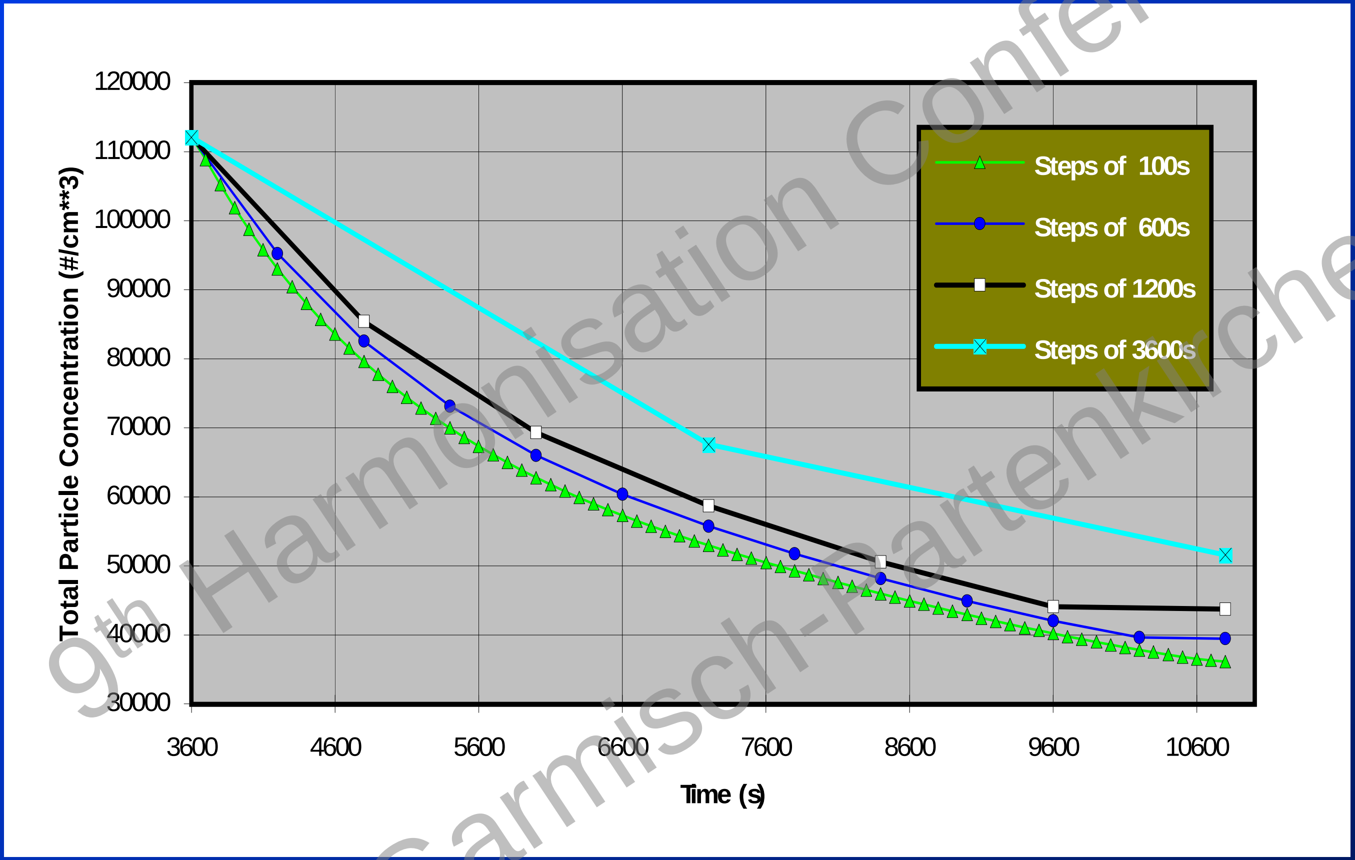

Minimum changes with steps up to 20 min

Influence CPU time on Particle Classes

Steps of 50s	CPU/REAL-Time Ratio
70 Classes	1.4E-03
50 Classes	8.8E-04
30 Classes	4.3E-04
20+10 Classes	4.3E-04

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Influence of the CPU time on the size of the Time-Step

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30 Classes	CPU/REAL Time Ratio
Steps of 100s	1.94E-04
Steps of 600s	0.55E-04
Steps of 1200s	0.27E-04
Steps of 3600s	0.27E-04

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- **The CPU/Real-Time Ratio achieved is 100 times faster than a typical R-K solution scheme**
- **Large time steps maintain physical representation**

Final Remarks

- **30-50 size classes are sufficient for analysing the particle spectrum of 0.0004-0.5 µm.**
- **More classes are needed for the range of small particles up to 0.006 µm.**
- **The evolution of the size spectrum is sensitive to the nucleation rates assumed.**
- **Coagulation is a process that can be evaluated under very large time steps under constant nucleation rates.**
- **FIA^2PES^2 as an implicit algorithm avoids the limitations of standard numerical methods and is suitable to be used in a multi-volume system.**