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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Study of contrail microphysics in the vortex phase with a Lagrangian particle tracking model" *by* S. Unterstrasser and I. Sölch

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This is the reply to the comments of reviewer #1. The comments are repeated (bold font) for your convenience. Our answers are printed with regular fonts.

The main subject of this manuscript, the loss of ice crystal number in the vortex phase of an aircraft contrail, is a significant one because it can affect subsequent contrail properties and development lasting for hours. It is a topic that has been discussed in several previous papers but is complex enough that significant issues remain. The starting point here is a previous study in a series of three papers by the first author and colleagues that used simplified

microphysics and fluid dynamics to allow a large parameter space of contrail behaviour to be simulated out to times of several hours. This, in my opinion, contributed significantly to the published literature of contrail studies. The present work is far more limited in scope: using a more explicit microphysics scheme, but treating only a modest number of cases and only in the vortex phase. The main conclusion reached is essentially that the previous bulk microphysics scheme was inadequate to correctly predict the crystal loss in the vortex phase, the more explicit scheme here giving significantly different results. As the authors note in the introduction, this work is not the first to use more explicit microphysics for such simulations or to demonstrate the sensitivity of crystal number loss to the sophistication of the microphysics scheme. Given the extent of the first author's previous contrail studies, however, I think it is still useful to publish this work in ACP as a correction to the previous study, provided those corrections can be clarified. The parametric studies included "sensitivity tests to temperature, relative humidity, initial ice crystal number and size distributions" are of more questionable utility: at the qualitative level only the sensitivity to initial size distribution study really covers new ground and several shortcomings in the simulations leave the quantitative accuracy of the results in doubt.

Motivated by your comment (3), we reconsidered our definition of the standard scenario and repeated all simulation runs. So far the setup of the bulk model was equal to the one of Unterstrasser, Gierens and Spichtinger (2008) in order to allow for a direct comparison to the previously published results. As described in section 2 we use a special tool to assure a realistic vortex decay by locally increasing the diffusion coefficients around the vortices. So far the enhanced diffusion was applied to all model fields (except the ice phase in the LCM). The high diffusion coefficients were intended to mimic the enhanced dispersion rates expected in a fully three-dimensional approach. In the new model versions (bulk and LCM) the enhanced diffusion is only applied to the grid-scale velocity components u and w, which gives a more consistent transport of the ice crystals and the water vapour, especially in the LCM. The changes in the setup are described in a new paragraph in the beginning of section 2. Qualitatively the general findings of the study are not affected, however quantitatively new results are obtained. In order to quantify the implications on our results we added several figures to this comment. Figure 1 and Figure 2 show the temporal evolution of the fraction of surviving ice crystals mass and number, respectively, at $T^* = 217$ K for several relative humidity values in the present (dotted) and previous (solid) bulk model version. The type of plot is analogous to Figure 2 of the manuscript, where the bulk model is compared to the LCM, now with the updated setup. Differences in the mass evolution between the two bulk models are primarily caused by different water vapour diffusion coefficients. Apparently for high coefficients (old version), moist air is entrained into the primary wake at high supersaturation and the crystal mass grows for $t > 100$ s. In the new model version the water vapour entrainment into the primary wake is limited and the ice mass steadily decreases. Contrarily for low supersaturation the ambient air has a lower absolute humidity than the air in the saturated, yet warmer primary wake. Accordingly, the ice mass is higher in the present model version and also more ice crystals survive than in the previous model version. For the high supersaturations the number of surviving ice crystals is also higher in the new model version. This is due to the fact that less crystals are detrained.

Specific comments/revisions/questions:

(1) Given the main conclusion here, the authors should provide more explicit guidance on which new results from the previous recent study (Unterstrasser et al 2008, Unterstrasser and Gierens 2010a,b) in their opinion still stand, which are cast in doubt and which should now be retracted.

The strength of the previous paper was the scan of a large parameter space which allowed to investigate the relative importance of numerous parameters on the crystal loss. The significant sensitivity to relative humidity and temperature was confirmed with the LCM model. Moreover we extended the relative humidity up to 140% in the present work. In the LCM the impact of relative humidity is even larger than in BM. (see Conclusion, p. 14660, l. 1-8 of the old manuscript). As discussed we are not able to decide which results represent the truth, but to our opinion the crystal loss for high supersaturations ($RH_i > 120\%$) and cold temperatures ($T < 212$ K) may be overestimated in BM. However, these high supersaturations were not examined in the previous work.

We added several sentences in the discussion section to touch upon further aspects of the previous paper like the validity of the parameterisation formula and the sensitivity studies treating the impact of stratification and eddy dissipation rate:

In UGS08 the impact of the ambient turbulence and stratification was examined. Following Holzäpfel (2006), both parameters affect the lifetime of the vortex pair and its decay is slower in a less turbulent and/or less stable atmosphere. For supersaturations $RH_i < 120\%$ (as discussed in UGS08) the moderate sensitivity to both parameters should be present in the LCM as well (not simulated). Analogously to the RH_i-sensitivity also a more pronounced dependence can be expected in the LCM. The number loss rate $f_{\mathcal{N},\mathrm{tot}}$ has a steeper gradient in the LCM once the sublimation has started and thus a shift of t_{breakup} affects the extent of the crystal loss more strongly than in the BM. For high supersaturations and lower temperatures the crystal loss is generally less critical, the number and mass loss rates are smaller and thus a moderate change in t_{breakup} has a limited effect on the eventually surviving fractions.

In this rather crude sense, the parameterisation of $f_{\mathcal{N},\text{tot}}$ with a power law relationship (see Eq 5.1 of UGS08) remains valid within the specified parameter range ($T = 209 - 222$ K and $RH_i = 120\%$). For $RH_i > 120\%$ one may extend the functional relationship in a linear manner, obeying continuity at $RH_i = 120\%$ as already done in Kärcher et al., 2009. There it was assumed that $f_{\mathcal{N},\text{tot}}$ linearly increases to 75% at $RH_i = 150\%$. In consideration of the new findings with the LCM model, we recommend to use 100% as maximum value for $f_{\mathcal{N},\text{tot}}$ at the upper humidity limit.

(2) In the previous bulk microphysics model the crystal loss was treated with an ad hoc parameterisation with some particular choice of exponent (Eq. 5 here). The particular comparison results here are thus not valid for bulk models in general but just for that particular choice and this should be made clear in the abstract and conclusions.

That's a good point. We added some lines in the beginning of section 3:
We want to emphasise that several particular comparison results only hold for the two specific microphysical models used here and cannot be generalised to any pair of Lagrangian-based and bulk model. Especially the two-moment bulk model results depend on the choice of the sublimation parameter α as outlined in section 1.3.
and in the Conclusion to clarify this:
We note that this particular comparison result cannot be generalised to other bulk models.
We do not think it is necessary to mention it in the Abstract, as no particular comparison results are mentioned there.

For example it is not a general feature that two-moment bulk microphysics overestimates the crystal number loss relative to size-resolved microphysics as is found here; the earlier study of Huebsch and Lewellen showed the opposite, for example, in comparing results of a different two-moment bulk microphysics with size-resolved results.

Lewellen & Lewellen underestimated the number loss, since they used a monodisperse size distribution and ice crystals in a grid box are only lost, if the ice mass totally sublimates within the grid box. Although in our bulk model the parameterisation of the sublimation process does not use the parameters of the underlying lognormal distribution it has motivated the inclusion of the fractional crystal loss. Depending on the choice of α we can "generate" cases where the bulk model prognoses more or fewer ice crystals to survive the vortex phase. One might implement the sublimation parameter α as a function of ambient humidity, the mean crystal mass/diameter or width of the size distribution. Anyway, you could not justify the choice by physical reasons. Once the LCM was operational there was no need to improve the sublimation parameterisation of the bulk model. Imagine we would find a function for α such that the bulk results match the LCM much better, it is still not clear whether the bulk model was generally improved or only for this special application.

It would be useful if the authors could discuss whether it might be possible to alter bulk models to give a more correct prediction of the crystal loss or whether there is some fundamental limitation preventing such correction.

In order to clarify this point we added to the discussion: *Gierens and Bretl (2009)* *discuss the sublimation parametrisation issue in two-moment bulk models. Testing the sublimation parametrisation against an analytical solution of the growth equation they found that there is no unique function relating crystal loss to mass loss. This reveals a fundamental limitation to ultimately correct a two-moment bulk model. Since sublimation is a dominant feature in the simulation of the vortex phase a Lagrangian treatment of the ice phase or size-resolved microphysics should be applied.*

(3) There are serious issues involved in providing a consistent treatment of turbulent diffusion in a mixed Eulerian-Lagrangian model. How have the authors insured that the terms added to include turbulent dispersion to the Lagrangian treatment of ice advection (mentioned in line 25 p14646) give dispersion rates consistent with those computed for water vapour (or perhaps total water) in the Eulerian framework? Discrepancies between the two can in some formulations lead to spurious changes in ice growth/sublimation. Also, some of the differences between the "bulk" and "explicit" microphysics simulations here (e.g., the changes in total IWC) are due largely to changes in the dispersion treatment rather than the microphysics; the authors should clarify how much of the changes seen in crystal number are due to this source rather than solely microphysics as is implied.

We agree with the reviewer that a consistent treatment of turbulent diffusion in a mixed Eulerian/ Lagrangian two phase flow approach is a serious issue. We now specify our treatment of turbulent ice crystal dispersion in section 2.2 and added: *For the calculation of the trajectories of an individual SIP an additional turbulent velocity component is added to the grid scale velocities. This accounts for turbulent dispersion of the ice crystals. The standard deviation of these velocities is taken to*

be proportional to the turbulent kinetic energy per unit mass, which is prognosed in the EULAG model and is, therefore, consistent with the subgrid scale closure scheme of the underlying dynamical core. Additionally the turbulent velocity components are assumed to be autocorrelated over the Lagrangian time scale. Unavoidable numerical diffusion in the Eulerian transport of the water vapour may lead to slight discrepancies in the dispersion rates for ice and the water vapour field. However, it is not necessarily true that these dispersion rates have to be the same, due to the inertia of the ice crystals and their relative motion to the sourrounding air by sedimentation..
The extent of detrainment into the secondary wake is moderately larger in the BM than in the LCM model. Since the majority of ice crystals remains inside the vortex system (as confirmed by Paugam et al., see also answer to point 6) the influence of the different dispersion treatments on the evolution of the ice crystal number concentration in the primary wake should be small. Accordingly, the results for the total number fractions of surviving ice crystals in both models for $RH_i < 120$% are in closer agreement now. Thus, differences in the old comparison should have been attributed to the different dispersion rates as well. For the present comparison the differences can be largely attributed to the microphysics.

(4) The term "large-eddy simulation" (LES) implies that the most important dynamics being considered is modeled by the Navier-Stokes equation, resolved on the chosen grid. Given that the treatment here is (a) strictly 2D and (b) the decay/diffusion of the vortices is artificially imposed rather than simulated it is not appropriate to refer to the treatment as LES. Also, given the fall of the vortices during the simulation and the influence of line vortices at large distances, the small domain size chosen (relative to the vortex spacing) may adversely affect the simulations (unless perhaps the boundary conditions ?unspecified in the text ? are particularly sophisticated).

It is true that we should not use the term LES. We replaced it by high resolution numerical simulations. As the vortex sinking and decay is imposed by artificially increasing the diffusion the boundary conditions should have no substantial impact on the results. In order to confirm this we carried out a LCM-simulation with doubled vertical and horizontal domain size or periodic instead of open boundaries. We found that the main characteristics of the vortex decay (like circulation evolution, descent speed and final vertical displacement) practically do not change, i.e. the vortex adjustment tool works and the chosen domain is adequate. Consequently the microphysical quantities differed only slightly from the according default simulation with $RH_i = 120\%$ and $T = 217$ K, e.g. the absolute difference in the fraction of surviving ice f_n is less than 0.5%. We added at the beginning of section 2.4: *Open boundaries are chosen in the lateral direction. Sensitivity studies with a doubled domain size or periodic boundary conditions do practically not change the results and the chosen conditions are suitable.*

(5) The early part of the vortex phase is not simulated, but rather an idealised velocity profile is prescribed, with a very crude initialisation of the ice crystal spatial distribution superposed (uniform 20m radius disks surrounding the vortex cores). Simulations of the earlier phases (by several groups) particularly of the engine exhaust dispersion/roll-up does not give distributions like that shown in fig.1. How does this affect the quantitative results later on? The results shown for sensitivities to initial ice crystal number and size distribution can both be expected to be strongly influenced by this choice of spatial initialisation.

We assume that the vortices are fully rolled up at our initialisation time. As done in

many other numerical wake vortex studies we initialise the tangential velocity with an analytical radial profile.

We carried out several sensitivity studies with different spatial distributions. The default simulations used 20m-circles with uniform concentrations. As the spatial distribution may affect the detrainment rate and the area of the primary wake, we carried out simulations with other spatial distributions. To keep it simple we only used uniform distributions, however the location of the ice crystals is strongly modified:
a) Uniform concentration inside a circle with $R = 10$ m (green curves)
b) Uniform concentration inside a circular ring from $R = 5$–15 m (brown curves)
c) Uniform concentration inside a circular ring from $R = 10$–20 m (blue curves)
d) Uniform concentration inside a circular ring from $R = 15$–25 m (purple curves)

Clearly, the concentration level was set inversely proportional to the initial area in order to leave the initial total number unaffected. The results are shown in Figure 3. Not surprisingly, the extent of the secondary wake is affected by the spatial distribution. The secondary wake is very weak for spatial distributions a) and b) and we do not think these are adequate initialisations. For the three remaining distribution types (standard, c) and d)) between 4% and 10% of the ice crystals are part of the secondary wake. Consistently, the fraction of ice crystals is lower in the primary wake the more crystals are detrained. Despite of the different detrainment, the total number of surviving ice crystals is pretty similar for the chosen ambient conditions.

The total ice mass attains different maximum values as the amount of water vapour depositing on the crystals scales roughly linearly with the cross-sectional area of the contrail. After ~ 80–90 s the added water vapour has sublimated into the air again independently on how much of it was added before. The subsequent ice mass evolution is similar.

We rerun the sensitivity studies for the width of the initial size distribution and the initial ice number concentration at $T^* = 217$ K and $RH_i = 120$% with different initial spatial distributions of the ice crystals. Figure 4 and 5 show the according sensitivity functions $f_{r,\mathrm{norm}}$ and $f_{\mathcal{N}_0,\mathrm{norm}}$ (case c (dashed); case d (dotted)). Although the extent of the secondary wake is strongly affected by the choice of the spatial distribution, as mentioned above, the functions $f_{r,\mathrm{norm}}$ and $f_{\mathcal{N}_0,\mathrm{norm}}$ nearly coincide for the standard runs and the runs with altered spatial distributions. Thus, the sensitivity to the ice crystal number concentration and width of the size distribution clearly dominates and the results obtained hold irrespective of this additional uncertainty. We added to the manuscript:
The sensitivity to r was tested for various spatial initial distributions. In further simulations the initial ice crystals are uniformly distributed inside a circular ring between the radii $10 < R < 20$ m or $15 < R < 25$ m and the sensitivity to r was very similar to the runs with the standard spatial distribution (not shown). Thus, the sensitivity to the width of the size distribution clearly dominates and the results obtained hold irrespective of this additional uncertainty.

(6) The results given for the "secondary wake" in several places in the paper seem on particularly poor footing given that the fraction of crystals ending up in the secondary wake will depend not only on the initial distributions but on the turbulent mixing/ detrainment of the "primary wake", both crudely treated here. This implies a corresponding uncertainty on the statistics of the primary wake as well.

We think the evolution in the primary wake is not that much affected. Let's assume two cases with maximal ice crystal number fractions of 5% and 15% in the secondary

wake, then the primary wake maximally consists of 95% and 85%, respectively. The relative difference in ice crystals number and concentration in the primary wake is small ($0.95/0.85 = 1.12$), especially when it is compared to the range of initial numbers of crystals $[0.1 - 10]$ covered in the sensitivity study shown in section 3.4. From this sensitivity study follows that the microphysical evolution should be very similar for the two hypothetical cases for the ratio 1.12.

(7) The comparison invoked with the 3D results of Paugam et al. to bolster the detrainment results here and support the 2D treatment (line 25 p14658 and line 26, p14660) is not very effective because Paugam et al. use a quite different (but also idealised) starting point (Gaussian distributions of crystals centred on the vortices rather than uniform spots) as well as a different stratification level. Likewise in the earlier comparison with 3D results of Huebsch and Lewellen the conditions are not close to being matched so that the conclusion cited from that comparison here (line 23 p.14642) is not supported except in a very crude sense.

We admit that stratification affects the detrainment rate and Paugam et al. used a more stable atmosphere than we do. The sensitivity study presented at point 5 revealed that the initial spatial distribution clearly has an impact on how many ice crystals eventually belong to the secondary wake. Despite the fact that Paugam et al. use a quite different spatial distribution they also end up having around one tenth of ice crystals in the secondary wake. Although you may claim it a crude comparison we feel confirmed that it serves our purpose, i.e. to state that the majority of ice crystals remains inside the primary wake.

Concerning the sparsity of different atmospheric conditions generally studied with the published 3D-models and the microphysical flaws in the model of the early Lewellen and Lewellen paper, the comparsion with Huebsch and Lewellen was the best one could do. We think the atmospheric and aircraft parameter agree fairly well for the compared simulation runs, and we would rate it a fair comparison.

(8) Why do the results given in fig.7 seem discontinuous between RHi 110% and 105%? The former results lie above those from RHi = 120% and increase with decreasing r, the latter lie below and decrease. The words in the text (line 14 p14655) need to be made consistent with the situation as well.

Please note that in the new manuscript the description of the r-impact was modified. It turned out that the reversed effect as observed for $RH_i = 105$% in the old manuscript now only occurs for very few $T - RH_i$-combinations of our parameter space (warm and slightly supersaturated). Basically, the reversed relationship occurs only if very few ice crystals survive and thus the absolute changes in the prognosed number of surviving ice crystals are rather small. Regardless of this modification the general statement that the problem of quantifying the crystal loss intensifies if the ISD are smaller definitely holds. We explain in the manuscript by:
For very dry conditions and a relatively high temperature at cruise altitude ($\mathrm{RH}_i^*=100\%$ *and* $T^*=222$ *K) the effect of a* r*-variation is opposite to the latter case. This means that the fraction of surviving ice crystals is largest when the ISD is broad and fewer crystal survive for a narrower ISD. Generally in a drier environment more crystals are lost. All crystals initially belonging to the left part of the SD will be lost anyway for all* r*'s and only initially large crystal are likely to survive the vortex phase. Since a broader distribution has more larger particles than a narrow distribution, more crystals survive in this case. Contrary to the latter case with* $T^*=217$ *K now the shape/position of*

the right part instead of the left part of the ISD is significant for the crystal loss. Although it seems to be a rather rare phenomenon in the present study, in ambient situations supporting longer vortex lifetimes and a larger vertical displacement of the vortex system this situation might occur more often. Moreover, a change in aircraft geometry/mass and water vapour emission can favour it as well.

(9) Is it purely a coincidence that, after quite different time evolutions, the BM and LCM results end at the same points for the RHi = 105% and 110% cases in fig. 2?

Yes, one may call it a coincidence that for each of the two RH_i-values the curve of the bulk and LCM model intersect each other for the specified $t_{breakup}$. In the new manuscript with the updated simulation results the BM and LCM curves end up at the same point for RHi=120%.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 14639, 2010.

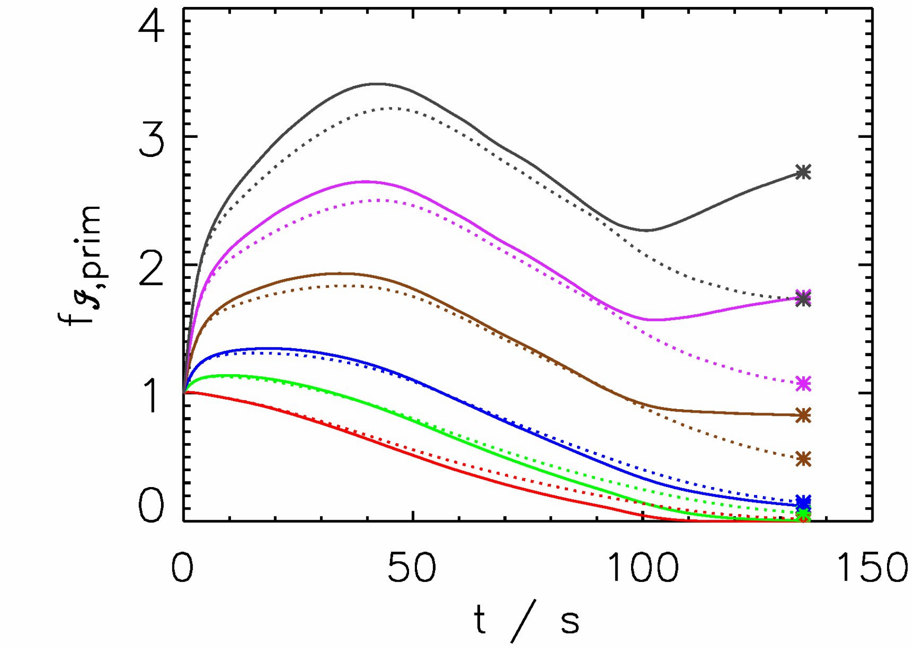

4
3
2
1
0
$f_{\mathcal{G},prim}$
0
50
100
150
t / s

Fig. 1.

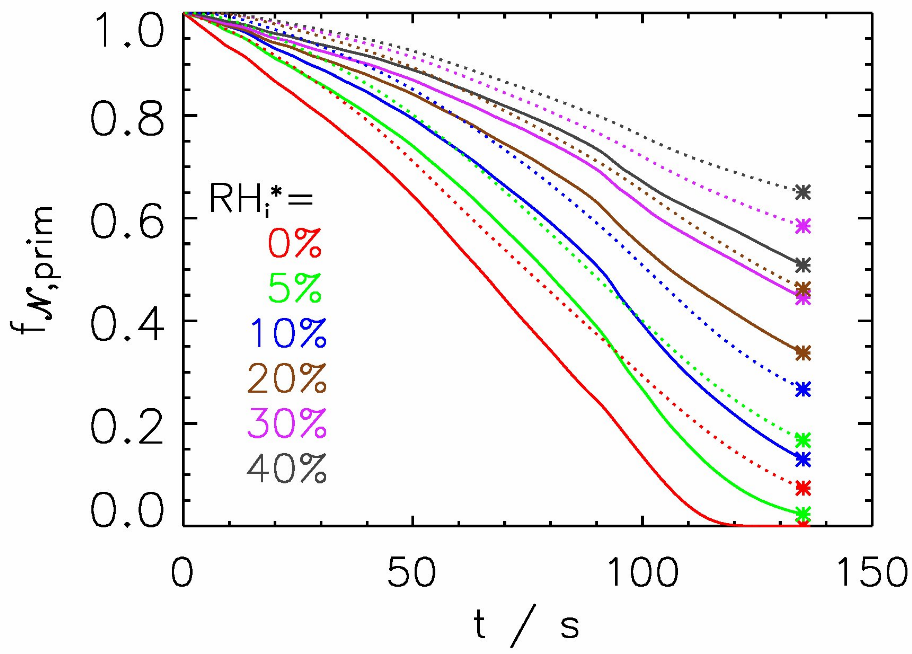

1.0
0.8
0.6
0.4
0.2
0.0
$f_{\mathcal{N},prim}$
RH$_i$*=
0%
5%
10%
20%
30%
40%
0
50
100
150
t / s

Fig. 2.

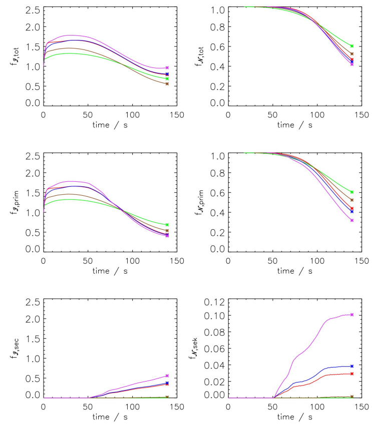


Figure 1: Ice mass and crystal number evolution at T=217K and $RH_i = 120\%$ for various spatial distributions (LCM). Circle with r=20m (default): red; circle with r=10m: green; circular ring from r=5 to 15m: brown; circular ring from r=10 to 20m: blue; circular ring from r=15 to 25m: purple.

2

Fig. 3.

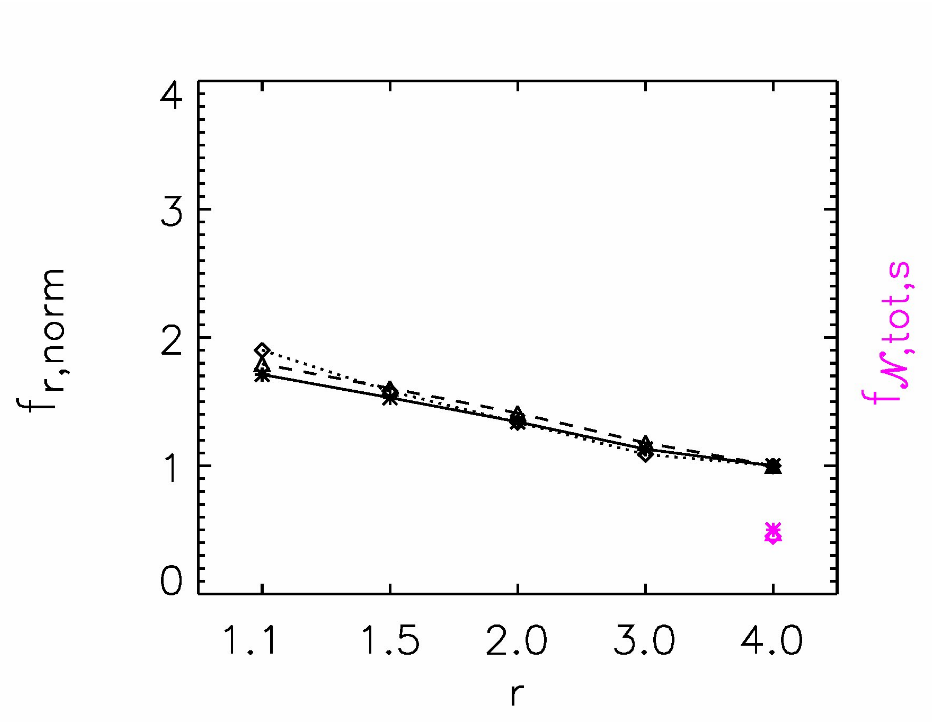
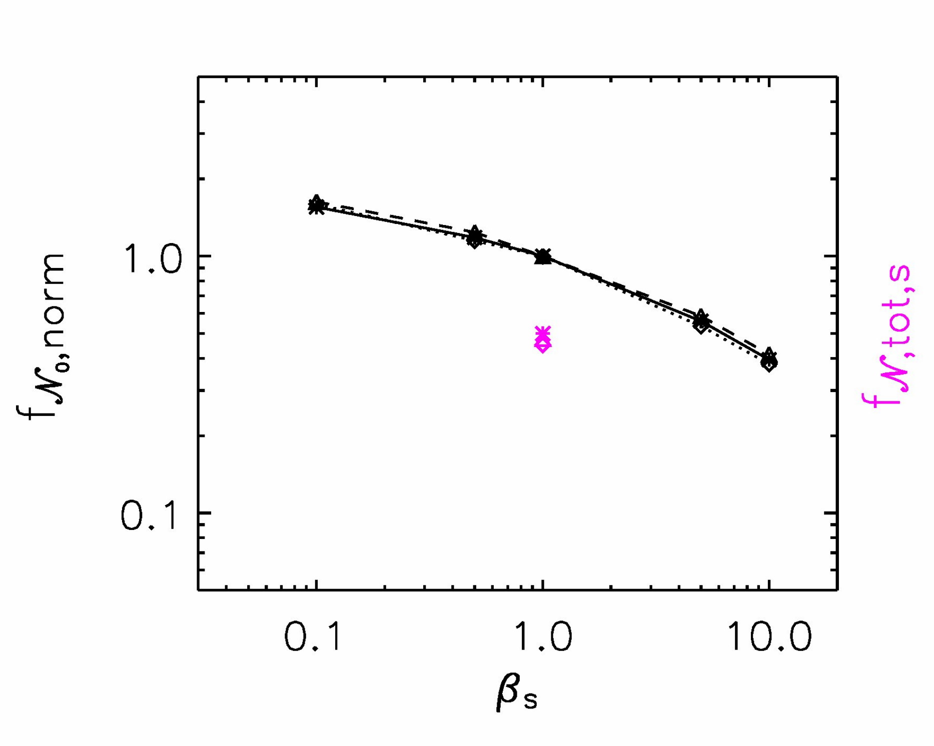


Fig. 4.



1.0
0.1
0.1
1.0
10.0
$f_{\mathcal{N}_0,\mathrm{norm}}$
$f_{\mathcal{N},\mathrm{tot,s}}$
β_s

Fig. 5.