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Interactive comment on "PLUME-MoM 1.0: a new 1-D model of volcanic plumes based on the method of moments" *by* M. de' Michieli Vitturi et al.

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PLUME-MoM 1.0: A new integral model of volcanic plumes based on the method of moments

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Responses to Referee 1

Dear Referee, thank you very much for the thorough review of the manuscript. You can find below the reply to the comments and a revised version of the manuscript where we have highlighted the changes and the new text added to clarify the points raised by the referees. Please note that some additional details can be found in the answers to the other referees.

R1. *Title and pg 3746 ln 2: The description of the model as 1-D is misleading. The model gives three-dimensional results (the wind can change direction and, with a model for the radial variation of the fields, the three dimensional character of the plume can be reconstructed). Rather, the model has only 1 independent variable, the arc-length* *along the centreline. It would be better to describe the model as an integral model, as it is derived by integrating the point-wise conservation equations over the plume cross-section.*

A. We agree with the suggestion of the referee. We removed 1D from the title and the text and the model is now described as an integral model.

R1. *Pg 3749: How are the moments defined in equation (1) related to other descriptions of the shape of the distribution such as the mean, variance, skewness, kurtosis? Could central and standardized moments be used to make this connection between descriptions of the distributions?*

A. The central moments can be expressed as terms of the raw moments (i.e., those taken about zero) using a binomial transform. In this way it is also possible to relate the moments of the distribution with the mean, variance, skewness, kurtosis. We added a sentence to clarify this fact in the manuscript at the end of section 2.1.

R1. *Pg 3749 ln 17: Does the prefactor in M(3) assume spherical particles? Can the same interpretations of the moments be made if the particles are not spherical, as is typical for volcanic pyroclasts? I recommend writing π/6M(3) j = α s,j as α s,j is used subsequently.*

A. The referee is correct: the prefactor assumes spherical particles and this is now clarified in the text. For particles with different shapes, if volume scales with the third power of length, we can relate the particle volume V and particle length L through a volumetric shape factor kv: V=kv L3. it is possible to introduce a sphericity parameter to relate the diameter with the particle volume.

R1. *Pg 3752 equation (7): The quantities k 1 , k 2 , k 3 are not defined and their values are not given. Dimensional analysis shows that their dimensions differ – do these quantities have a physical meaning? Also, C D should be defined and the used value given.*

A. The values of the different parameters have been added to the text.

R1. *Pg 3753 equation (10): It appears that there has been an implicit definition the square bracket notation as*

$$[g(D)]^{(i)} = \frac{1}{M_j^{(i)}} \int_0^{\infty} g(D) f_j(D) D^i dD.$$

It would useful to make this definition explicit, as it is used subsequently. Also, as the denominator in equation (10) doesn't depend on D it can be taken out of the integral.

A. The definition of the moments of other variables is at page 3750, Eq. 2 (of the original manuscript). The square brackets are used in Eq. 10 (of the original manuscript) because the moment appearing on the right-hand side is not the moment of a single variable but the moments of the product of two variables. The denominator has been taken out of the integral.

R1. *Pg 3754: the use of two variants of the phi symbol (ϕ and φ) (one used for the phi-scale size and the other for the particle mass fraction distribution) is not a very convenient notation.*

A. The variable γ is now used for the particle mass fraction distribution.

R1. *Pg 3754: it should be explicitly stated that* $\Pi_j^{(0)} = x_{s,j}$.

A. It is stated in the text that "the moment $\Pi_j^{(0)}$ is the mass fraction of the $j-$th solid phase $x_{s,j}$ with respect to the gas-particles mixture"

R1. *Pg 3754 equation (13): there is another use of the square bracket notation, but this is inconsistent with the previous use (see comment 5). In particular, the kernel and variable of integration differ in these definitions. A new notation is needed.*

A. As stated before, the square bracket are not used for any particular notation. The notation used here is only the superscript (0) for the moment of the heat capacity.

In any case, the square bracket is superfluous in Eq. 13 (of the original manuscript) and also the denominator in the right-hand side should be removed, as well as the denominator in the right-hand side of Eq. 14 (of the original manuscript).

R1. *Pg 3755 ln 5: ϕ is used to denote an angle, but it has previously been used to denote the particle size. x has also been used previously.*

A. A different notation has been introduced for the angle, while we do not think that there are problems with the similar notations used for the horizontal coordinate x and the mass fraction x_{sj}.

R1. *Section 3: There are numerous assumptions implicit in the equations presented. These assumptions must be made explicit.*

A. The assumptions have been made explicit in the text adding the following lines: "The model assumes an homogeneous mixture of particles and gases with thermal and mechanical equilibrium between all phases. Aggregation and breakage effects are not considered here and consequently density does not change with time. Finally, the model does not consider effects of humidity and water phase changes."

R1. *The symbol α has already been used.*

A. A subscript has been added to the symbols used for the two entrainment coefficients.

R1. *The entrainment formulation given in equation (20) was first proposed by Hewett et al 1971 (http://dx.doi.org/10.1016/0004-6981(71)90028-X). This reference should be used.*

A. The suggested reference has been added.

R1. *Pg 3737 ln 19: The text states that the equations for the conservation of momentum (equations 22 and 23) can be derived from the conservation of mass (equation 21). This is not correct – independent information is required (Newton's second law). This also applies to the similar discussion on pg 3761.*

A. The text has been corrected and now it states: "From Newton's second law and the variation of mass flux ...".

R1. *Pg 3758 ln 18: The bulk densities ρ^B_{atm} and ρ^B_{wv} are not defined. Need to state how ρ_g is determined from the bulk densities.*

A. The definitions of the bulk densities have been added to the text: "bulk density of the particles of the j-th family (i.e. the mass of particles of the j-th family per unit volume of gas-particles mixture)".

R1. *Pg 3759: The derivation of the rate of change of the mixture specific heat capacity is not clear. Why are partial derivatives used (what variables are held fixed)? Why is the second term on the right-hand-side written in this way?*

Pg 3760 lns 7-10: Does the use of ρ_{mix} and C_{mix} at s to find T at $s+ds$ result in a first-order scheme? I suggest removing these lines as the direct integration of equations (28) and (30) are preferred?

A. The partial derivatives have been changed to total derivatives. Eqs. 28 and 30 have been added to close the system of equations and to avoid, as stated in the text, the use of ρ_{mix} and C_{mix} at s when calculating the updated variables at $s+ds$. Without the new value of C_{mix}, given by Eq. 30, it is not possible to find the value of T at $s+ds$ from the solution of Eq. 24 only. In the same way, the updated value of the gas constant is needed to compute the new density at $s+ds$. In any case, the text has been rewritten to clarify this fact.

R1. *Section 4.1: There is extensive use of jargon in the description of this algorithm that results in a lack of clarity. In particular:*

(i) the term "realizable moment set" should be avoided or defined.

(ii) the term "invalid moment set" requires clarification.

(iii) what is "moment corruption" and how can it be diagnosed?

(iv) Hankel-Hadamard determinants require definition or reference.

(v) why do nodes within the support of the distribution and positive weights guarantee accuracy of the algorithm? An explanation and reference are required.

(vi) it not clear at which point in the predictor-corrector numerical integration the algorithm is used. Is it in both the predictor and corrector step?

A. (i) the definition of "realizable moment set" is given at lines 20-21: "meaning that there exists a particle size distribution resulting in that specific set of moments". In any case, we moved it after the first use of the term "realizible" to make it clearer.

(ii) the sentence has been removed.

(iii) the following text has been added: "the problem of moment corruption (i.e. the transformation during the integration of the moment-transport equations of a realizable set of moments into an unrealizable one)"

(iv) a reference to Gautschi, 2004 has been added

(v) a reference has been added.

(vi) the algorithm is used in both the predictor and corrector step. This has been clarified in the text.

R1. *Pg 3765 ln 1: "The initial moments are evaluated analytically..." This can only be true if a probability model is provided for the initial particle distribution and the model is sufficiently integrable to calculate the required moments.*

A. The sentence has been changed stating that the moments are evaluated analytically for the initial particle distribution presented in this work. We remark here that the distributions considered in the paper are not probability densities and the integral over the size spectrum can be different from 1.

R1. *Pg 3765 lns 4-8: This paragraph is not clear. I'd recommend re-writing, perhaps*

including the equation for $\varphi(\phi)$ given in equation (53) moved to this point.

A. Equation 53 has been moved as suggested by the referee.

R1. *Pg 3768: The justification for using the formulation based on the moments of mass fraction distribution rather than the number distribution (i.e. that the first three moments can be combined to give the mean and variance of a normal distribution) seems weak. Surely it is natural to use the moments of the particle mass fraction distribution to track changes in quantities derived from and describing the mass fraction distribution.*

A. It seems to us that what is written in the text is exactly what the referee says, i.e. that it is natural to use the moments of the particle mass fraction distribution to track changes in quantities derived from and describing the mass fraction distribution:

"when we want to track the changes of the mass fraction averaged diameter and its SD (or variance) in the ϕ scale during the plume rise, it is preferred to use a formulation based on the moments $\Pi^{(i)}$".

We also remark that the first three moments can be combined to give the mean and variance of any distribution, not only of a normal distribution.

R1. *Section 5.3: It should be noted that the sensitivity analysis performed is only a partial sensitivity analysis. Only a small subset of the model parameters and inputs are varied. The sensitivity results are therefore conditional on the values taken for the fixed parameters. In particular, it is possible that different inferences might be made if some of the fixed parameters take different values.*
gPCE: The generalized Polynomial Chaos Expansion is more similar to a spectral method rather than a finite element method, as the expansion is a high order polynomial posed on the whole domain of the input variable rather than a series of low-order polynomials each posed on a collection of subset (elements) covering the input domain. The multidimensional integral referred to on pg 3773 should be given or references provided - as written it is not clear how to determine the expansion coefficients, and there

are several methods for doing this. A reference is needed for Clenshaw-Curtis quadrature. It should also be noted that the requirement to evaluate multidimensional integrals might result in a high computational cost when there are a large number of inputs and when the integrand is not well behaved.
Pg 3774: When comparing the LHS and gPCE approaches, there is a choice of using 1000 and 2000 samples for the LHS. It would be useful to show small sample sizes for the LHS, to give a suitable lower bound on the number of samples. In particular, as the response surfaces found here are very smooth and with small variation, it is possible the smaller LHS would give good results here.

A. We agree with the referee that we are not presenting a full sensitivity analysis, but this is out of the scope of the paper. In the manuscript we want to present a plume model based on the method of moments, and one of the main advantages of the method is the capability to track in an effective way the changes of the mean and standard deviation of the particle distribution (with 4 moments only with the formulation based on the mass fraction). For this reason we presented a sensitivity analysis based on the uncertainty on these two parameters described by the moments.

Regarding the gPCE, we added the following reference to clarify the similarities with finite elements:

"R. Ghanem and J. R. Red-Horse. Propagation of probabilistic uncertainty in complex physical systems using a stochastic finite element technique. Physica D, 133:137–144, 1999."

Another reference has been added to clarify how the expansion coefficients are calculated and how the Clenshaw-Curtis quadrature is used:

"Eldred, M. & Burkardt, J. Comparison of non-intrusive polynomial chaos and stochastic collocation methods for uncertainty quantification AIAA paper, 2009, 976, 1-20"

For the comparison of the LHS and gPCE approaches, the number of runs has been

chosen using the values suggested in the DAKOTA user manual. We have done additional tests with a smaller sample size (500 simulations) and we report here the results for the cumulative distribution function of the Solid Mass Flux Fraction Lost (see figure above). UQ results clearly show the error in using 500 runs and that a large number of simulations (≥ 1000)is needed to reach a convergence of the results when the LHS approach is adopted.

R1. *Section 5.4: (i) The details of the sensitivity analysis should be given, or suitable references provided (e.g. Saltelli's Sensitivity Analysis book, Sobol' and Saltelli's papers on this topic). (ii) The technical definitions in terms of variance of the conditional expectation are not intuitive to non-statisticians.*

A. A reference to the following book has been added:

Saltelli, A.; Ratto, M.; Andres, T.; Campolongo, F.; Cariboni, J.; Gatelli, D.; Saisana, M. & Tarantola, S. Global sensitivity analysis: the primer John Wiley & Sons, 2008

R1. *Conclusion: Although only 91 simulations are required in the gPCE method applied to the plume model, I suspect that if the response function where not as smooth and well-behaved as for this model, many more model evaluations would be required. Furthermore, if more parameters were varied, the computational cost would increase for gPCE (and for LHS, although the advantage of gPCE might be reduced). Therefore, I feel there is an over-emphasis on the effectiveness of gPCE. In addition, is the computational saving enough to require the additional technical computations necessary? – there is a cost in code development time for gPCE that is significantly greater than LHS.*

A. The referee is right when he says that if more parameters were varied, the computational cost would increase for gPCE, and this is now stated in the text. Conversely, the computational cost of the gPCE is negligible compared to the cost of the simulations, and thus there are no significant advantages in using the LHS.

./figure-1.pdf

Fig. 1. Cumulative distributions and response surfaces for test Case 1 (weak plume without wind).

R1. *Figure 1: The cross-section of the plume is circular in a plane normal to the centreline of the plume. This isn't clear on the diagram.*

A. The figure has been modified accordingly to the suggestion of the referee. we hope the figure is clearer now.

R1. *Figure 2: The axes in the plots don't seem appropriate. The top plot has a range for the Particle number distribution from 10^{-50} to 10^{+50} , which seems extremely large. Furthermore, the top plot suggests there are particles erupted with diameter in excess of 10^7 m! I suspect the labelling of the axis has gone wrong (missing minus sign in the indices?) and the particle diameter decreases to the right? The phi scale labels are also wrong.*

A. The range for the Particle number distribution from 10^{-50} to 10^{+50} is correct, but the problem, as noted by the referee, is that on the x-axis the minus sign have disappeared, bot in the exponents of the diameters expressed in meters and the diameters expresses in the phi scale. The corrected figure is presented here.

R1. *Figure 6: A fair comparison of the two sampling strategies would be to have 81 points in LHS sample as well as the Clenshaw-Curtis grid.*

A. The number of points for the sampling strategies presented in figure 6 does not have any reference to the simulations performed but it has only been chosen to clearly present the strategies. Using 81 points with the LHS would mean to partition both the x and y axis in 81 stripes and it would make really difficult the readability of the figure. On the other side, using less points for the Clenshaw-Curtis grid would not highlight enough how the points are distributed in the domain.

R1. *Figure 9: The sensitivity indices displayed for the Top σ panels cannot be correct. The response surfaces in figure 7 and 8 show that the contours of Top σ are not absolutely parallel Bottom μ, so there must be some sensitivity to the Bottom μ.*

A. The sensitivity indexes are correct. We remark here that the fact that the subplots

./figure-2.pdf

Fig. 2. Schematic representation of the Eulerian plume model. The dashed black line represent the axis of the curvilinear coordinate s.

./figure-3.pdf

Fig. 3. Visualization of a normal initial distribution in the Krumbein ϕ scale for the solid particles.

in figure 7 and 8 are vertically stretched, and this could give the idea that there is a sensitivity to the parameter on the vertical axis larger than the real value. In any case the values of the sensitivity indexes, as computed from DAKOTA for Test case 2 and plotted in Figure 9 for "Top σ", are reported here:

```
Global sensitivity indices for each response function:



response_fn_2 Sobol indices:

                                 Main             Total

                     3.7227494471e-04  1.2250701556e-03 x1

                     9.9877492984e-01  9.9962772506e-01 x2

                          Interaction

                     8.5279521094e-04 x1 x2
```

We also report the coefficients of the polynomial expansion, from which it is possible to plot the contours and to evaluate analytically the sensitivity indices.

```
Polynomial Chaos coefficients for response_fn_2:
        coefficient   u1   u2
        ----------- ---- ----
   1.4336940817e+00   P0   P0
```



```
   1.6578858566e-02   P1   P0
  -2.5910899091e-03   P2   P0
  -2.8116627135e-03   P3   P0
  -3.2804547607e-04   P4   P0
   6.7952933063e-03   P5   P0
  -4.1395975864e-03   P6   P0
  -2.9026509458e-03   P7   P0
  -1.7098830327e-03   P8   P0
   8.9814284834e-01   P0   P1
   3.7262764551e-02   P1   P1
   7.5125408867e-03   P2   P1
  -1.6321040394e-02   P3   P1
   2.2132291023e-03   P4   P1
   5.8756408728e-04   P5   P1
   5.7838688541e-03   P6   P1
   1.1995615562e-03   P7   P1
  -7.4673637468e-03   P8   P1
  -4.1668082838e-02   P0   P2
   2.3065350042e-02   P1   P2
   2.3825461814e-03   P2   P2
   2.1148501070e-03   P3   P2
   1.7727374651e-03   P4   P2
  -8.8478841637e-03   P5   P2
   1.4551374661e-02   P6   P2
  -3.8051790789e-03   P7   P2
   1.8463422687e-03   P8   P2
  -4.0920148065e-03   P0   P3
  -1.6905356585e-03   P1   P3
  -4.9839259871e-03   P2   P3
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```
 3.8944263097e-03   P3   P3
 1.9329513445e-04   P4   P3
 1.0878441090e-02   P5   P3
-8.6680149485e-03   P6   P3
-2.2863854848e-03   P7   P3
-5.4586661825e-04   P8   P3
 2.2886609083e-03   P0   P4
-2.7465458556e-03   P1   P4
-3.0891928498e-03   P2   P4
-1.4646650257e-03   P3   P4
-4.7270771933e-03   P4   P4
 1.2163990228e-03   P5   P4
-1.3854824406e-02   P6   P4
 8.6678617316e-03   P7   P4
-6.7466120712e-04   P8   P4
 1.1657009672e-04   P0   P5
 4.9090095451e-03   P1   P5
 3.7946796588e-03   P2   P5
-2.9495112304e-03   P3   P5
-4.1482366786e-04   P4   P5
-9.5659085116e-03   P5   P5
 7.6261697982e-03   P6   P5
-2.9319826609e-03   P7   P5
 7.1749457251e-03   P8   P5
-5.7901135737e-04   P0   P6
-3.0281356063e-03   P1   P6
 4.2719008039e-03   P2   P6
 1.7583283179e-03   P3   P6
 8.3201878659e-03   P4   P6
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 2.6704665368e-03   P5   P6
 1.2441515329e-02   P6   P6
-4.0571117721e-03   P7   P6
-9.6858649511e-03   P8   P6
-1.0293447697e-03   P0   P7
-3.7909388725e-03   P1   P7
-3.4938230431e-04   P2   P7
 1.7733592128e-03   P3   P7
-4.2099940377e-04   P4   P7
 6.0366622193e-03   P5   P7
-7.3902454998e-03   P6   P7
 2.8979716727e-03   P7   P7
-5.2051392647e-04   P8   P7
 1.4606844135e-03   P0   P8
 7.3041710628e-03   P1   P8
-9.1532601056e-03   P2   P8
-9.8399168578e-04   P3   P8
-1.0310831209e-02   P4   P8
-6.2875060428e-03   P5   P8
-6.4367915934e-03   P6   P8
-6.2543284009e-04   P7   P8
 1.0071554844e-02   P8   P8
```

R1. *Technical corrections*

A. We have considered all the corrections suggested by the referee modifying the manuscript when appropriate.