A framework for systematic testing of an improved wet deposition scheme for the Lagrangian dispersion model FLEXPART

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Outline

• Motivation
• Objectives
• Testing procedures
• Outlook
## Motivation

1. **FLEXPART**
   - an important tool for the CTBTO

2. **Growing community**
   - parallel developments

3. **Software QA in science**
   - in general does not follow software testing standards

4. **(wet) deposition**
   - not yet operational at CTBTO, QA
Motivation: FLEXPART
Objectives

Goal

enhance credibility

robustness against wrong input

release

changes to the model

no

yes

finding bugs and problems

systematic testing

Goal

enhance credibility

robustness against wrong input
Testing procedures

„Program testing can be used to show the presence of bugs, but never show their absence!“

Edsger W. Dijkstra

... COMPLETE testing of software is not possible, BUT

Testing is „the process of operating a system or component under specified conditions, observing or recording the results and making an evaluation of some aspects of the system or component.“

ANSI/IEEE 610.12 standard
Code testing: static code analysis with FORCHECK

FORCHECK ...
• is a comprehensive Fortran verifier!
• locate bugs as early as possible during the development phase!
• helps to produce reliable and portable code!
• produces code metrics!

FORCHECK ...
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• helps to produce reliable and portable code!

e.g.  
1x[52 E] continuation character missing  
7x[312 E] no value assigned to this variable  
2x[484 E] invalid usage of value  
9x[506 E] multiple declaration of program unit or entry  
2x[563 E] number of arguments inconsistent with first occurrence  
2x[565 E] number of arguments inconsistent with  
7x[646 E] (MODULE NOT FOUND)  

number of program units: 145  
number of (sub)modules: 12  
number of module procedures: 18  
number of source files: 139  

number of error messages: 30  
number of suppressed messages: 2493
Code testing: systematic testing of input values

Test case: unrealistic input value

Value tested: total mass emitted

Value: 0

Result:
• no warning
• wrong particle number
Code testing: systematic testing of input values

Test case:  
optional input

Value tested:  
diurnal and annual  
variation of emission

Value:  
not specified

Result: 
• No warning  
• no particles released
Evaluation of results: visual inspection

Artifacts in the wet deposition fields

Reduced artifacts in wet deposition fields after enhanced diagnostics and interpolation of clouds
Evaluation of results: lifetime analysis

average climatological ratio $r$ of aerosol concentration $c_{lp}$ and noble gas concentration $c_{NG}$

removal of aerosols from the atmosphere

lifetime

Tihange is a NPP site in Belgium.
-> maritime climate

Almaraz is a NPP site in Spain.
-> Mediterranean climate.

NPP – nuclear power plant
Evaluation of results: statistical evaluation

1. carefully select data as reference for validating changes
   - real data
   - ideal data

   FLEXPART results (stable version)

2. compare
   - control result
   - test result

   statistical metrics

figure of merit in time/space
- percentiles
- correlation coefficient
- mean
- RMSE
- variance
- student-T

Courtesy: Don Morton and Delia Arnold
Conclusion/Outlook

Building a systematic and automated testing environment

• combine single components into one automated system

• establish benchmarks for comparison with future model developments

• special focus on wet deposition – relevant for CTBTO operational needs

• support a more effective model development within the community
THANK YOU!