Developing a fast photochemical calculator for an integrated assessment model

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Objectives

- Compare the implementation of two Photochemistry modules in a Lagrangian model.
- Test their performance in Integrated Assessment Models (IAM).

Conclusions

- Differences between the two methods increase with the time step.
- The use of a LookUp table (LUT) is suitable in the IAM framework since it fastens the calculation with acceptable accuracy.

Background

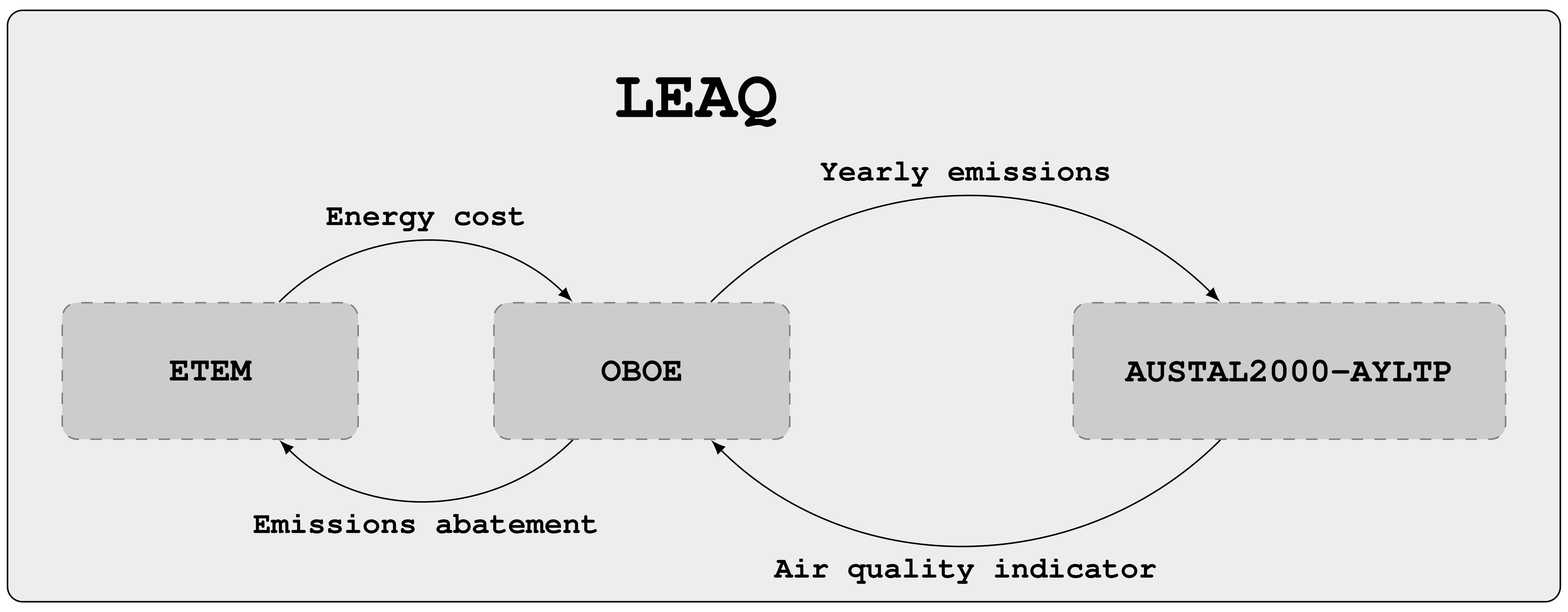

Figure 1: Overview of the IA - LEAQ model, the two sub-models and their relation.

- Air quality-IAM have two usages:
  - Simulation mode: 3D-eulerian models, CPU expensive, are useful to simulate abatement policies scenarios.
  - Optimization mode: faster models are required to find optimal measures which meet Air Quality standards.
- LEAQ is an air quality IAM designed for the Grand Duchy of Luxembourg [1]. It is composed of an energy model ETEM and an AQ model AUSTAL2000-AYLTP, linked by a master program running an optimization algorithm [2] (Figure 1).
- A photochemistry module has been implemented into AUSTAL2000 model for the LEAQ model.

Methodology

- We use quasi-linear reactions rates Ks to mimic the behaviour of ozone.
- Ozone has a non-linear behaviour, however we can assume that under a certain number of restricted conditions linear reaction rates holds.
- Two methods were applied:
  - AUSTAL2000 is plugged to the LUT to obtain the reaction rates.
  - AUSTAL2000 is plugged directly to OZIPR model. The reaction rates are not stored, but instead the current values of the variables are used as initial conditions to run OZIPR and the reactions rates are calculated immediately.
- In both methods the mass transformation is carried out by using the equations 1 and 2, for each species p, where c_p is the concentration, c' is the updated concentration, Δt is the time step, S is the domain and T, RH and θ are temperature, relative humidity and solar zenith angle respectively:

$$Ks_p(c_p(t), T, RH, \theta) = \frac{c_p(t+1, c_p(t), T, RH, \theta) - c_p(t)}{\Delta t}, \quad (1)$$

$$c'_{p,i,j,k}(t) = c_{p,i,j,k}(t) + Ks_p(c_p(t), T, RH, \theta)\Delta t, \ \forall(i,j,k) \in S, \quad (2)$$

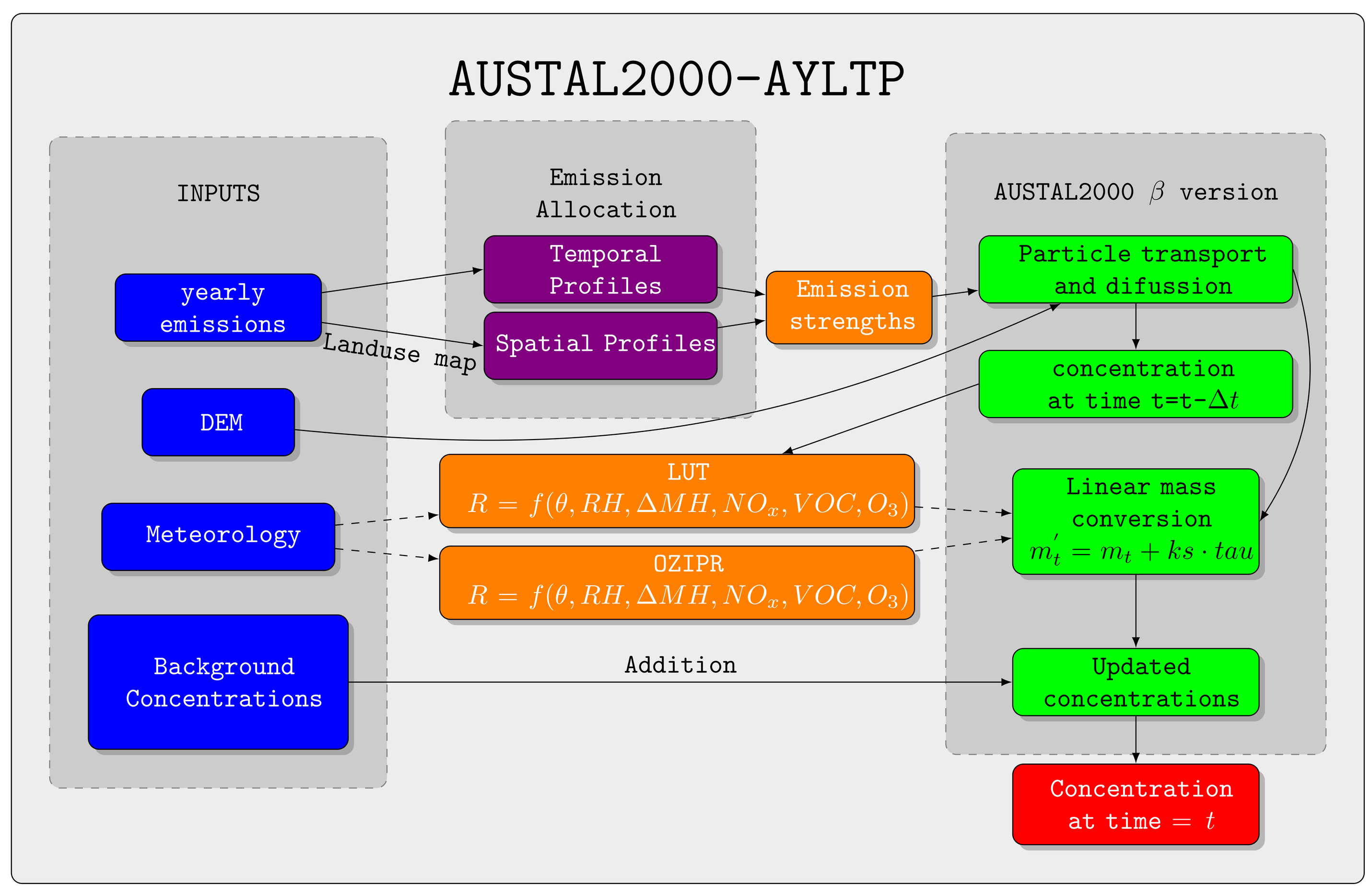

Figure 2: AUSTAL2000-AYLTP Structure, including both versions of the model represented by the dashed line. The photochemical modules represented by LUT and OZIPR blocks respectively.

Results and Discussion

Table 1: Simulation results of both model versions

Number of cells	Time step (min.)	CPU time (min.) LUT	CPU time (min.) OZIPR
25	10	4	78
120	10	9	96
480	10	11	184
120	60	3	419

Number of cells	Time step (min.)	Differences in average conc. [$\mu g.m^{-3}$]	Differences in average rates [$\mu g.m^{-3}.s^{-1}$]
25	10	0.000	0.0030
120	10	0.611	0.0017
480	10	1.643	0.0012
120	60	15.92	0.4540

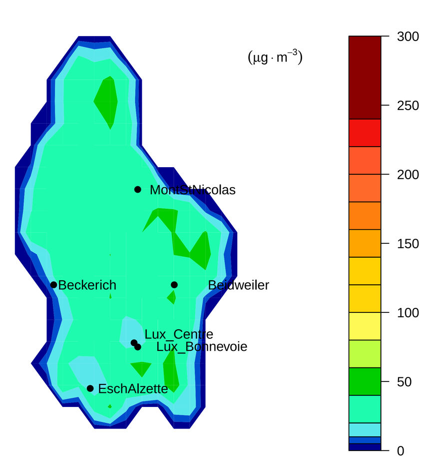

Figure 3: Modeled ozone concentrations ($\mu g.m^{-3}$) at 9 hours of 19-07-2006, the points represent the monitoring stations

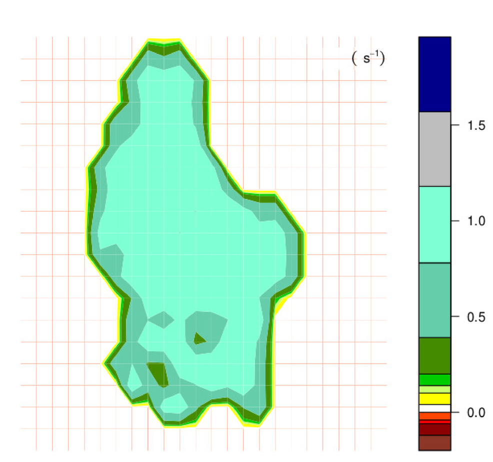

Figure 4: Spatial distribution of the ozone rates (s^{-1}), for the time step corresponding to 9 hours of 19-07-2006

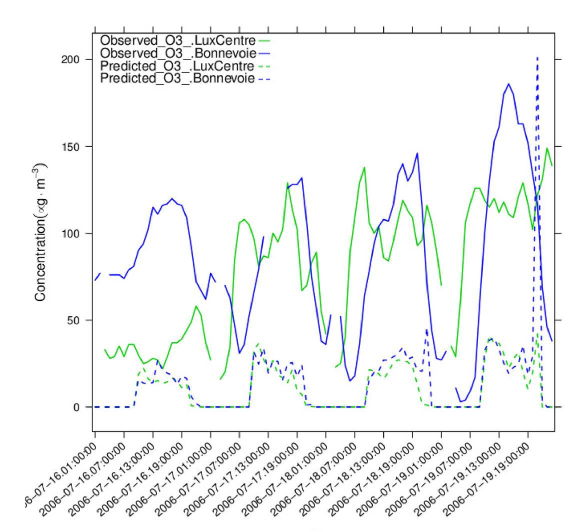

Figure 5: Comparison with the observed ozone values, using the stations of Bonnevoie and Luxembourg centre

References

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