Simulation of nitrogen behaviour of soil-plant systems

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4.14 A model to simulate partial anaerobiosis

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1. NAME OF MODEL

ANAER: Partial anaerobiosis in a model soil.

2. SYSTEM MODELED

A structured agricultural soil is represented by spherical porous equidimensional aggregates in a hexagonal packing with inscribed porous aggregates in its voids. For this geometry water and oxygen transport properties are modeled for the top 25 cm of the model soil in view of denitrification.

3. OBJECTIVE

To develop a mathematical approach to the problem of calculating partial anaerobiosis in structured soils taking into account the inter- and intra-aggregate water distribution, the oxygen transport from the atmosphere into the soil and from the inter-aggregate pores into the aggregates. Further to indicate deficiencies in the description of these processes in view of future research.

4. TIME SCALE

The model has been used to calculate the anaerobic soil volume before, during and after short rain periods. Total simulated time is one day and the time step used was 10^{-4} day.

5. DIAGRAM

ANAER is a model composed of the submodels water flow, macro diffusion of oxygen from the atmosphere into the soil, and oxygen diffusion from inter-aggregate pores into the aggregates. In the following the main processes are described.

Water flow: from functions relating water content to suction and hydraulic conductivity respectively, water flows are calculated following Darcy's law and subsequently used to calculate the new water content in each layer. The water flow submodel is based on a paper by Van Keulen & Van Beek (1971). Rain is introduced as a forcing function. Water uptake by roots is assumed to be homogeneously distributed over the profile. The ground water table is situated at a depth of 50 or 100 cm.

Macro oxygen diffusion: from a function relating diffusion efficiency to gas-filled porosity and from mass transport of oxygen out of the profile due to air displacement by rain water, oxygen flows are calculated and used to compute the new oxygen concentration in

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each layer.

Oxygen diffusion from inter-aggregate pores into the aggregates: functions relating water content to air-exposed area for each aggregate diameter, and to the equivalent radius of the water filled part of an aggregate were calculated. Diffusion of oxygen is taken proportional to air-exposed area, and the equivalent radius is used to compute its ratio to the critical radius at which just no anaerobiosis occurs. This ratio is used in the steady state solution to the diffusion equation for spheres to obtain the anaerobic aggregate volume (Currie, 1961). Respiratory activity is reduced in proportion to the anaerobic soil volume fraction.

6. LEVELS

See 5.

7. GOVERNING EQUATIONS

The equations describing the processes mentioned have previously been derived (Leffelaar, 1977, 1979). The interested reader is referred to the original texts.

8. INPUT PARAMETERS

a. *General inputs*
- radius of equidimensional aggregates, cm
- total pore volume, $cm^3.cm^{-3}$
- total depth of top layer, cm
- number of compartments.

b. *Water flow model*
- initial water contents, $cm^3.cm^{-3}$
- soil moisture characteristic
- hydraulic conductivity as a function of water content (calculated according Green and Corey, 1971)
- saturated hydraulic conductivity, $cm.d^{-1}$
- root water uptake, $cm.d^{-1}$
- depth of groundwater table, cm
- rainfall onset, intensity and duration as a function of time, d.

c. *Oxygen flow model for transport of oxygen from the atmosphere into the soil*
- diffusion efficiency factor as a function of gas-filled porosity (calculated according Millington and Shearer, 1971)
- diffusion coefficient of oxygen in air, $cm^2. d^{-1}$
- amount of oxygen in air, g $O_2.cm^{-3}$
- oxygen consumption rate at the moment that no anaerobic zones are present, g $O_2.cm^{-2}.25$ cm $depth^{-1}.d^{-1}$

d. *Oxygen diffusion from inter-aggregate pores into the aggregates*

- air exposed area as a function of water content for each aggregate diameter
- equivalent radius of the water filled part of an aggregate as a function of water content
- anaerobic soil volume fraction as a function of the ratio of the equivalent radius to the critical radius (calculated according Currie, 1961)
- distribution of the oxygen consumption over the aggregates
- diffusion coefficient of oxygen in pure water, $cm^2. d^{-1}$
- diffusion coefficient of oxygen in an aggregate, $cm^2. d^{-1}$ (calculated according Millington and Shearer, 1971)
- critical oxygen concentration at which it is stated that anaerobiosis occurs, $g\ O_2.cm^{-3}$
- relative solubility of oxygen in water.

9. OUTPUT; VERIFIABLE VARIABLES

- Anaerobic soil fraction as a function of time.
- Anaerobic aggregate fraction for each aggregate diameter.
- Oxygen concentration in the inter-aggregate pores.
- Water content.

10. OBSERVATIONS

The model was used to indicate which problems need more attention by performing a sensitivity analysis of the different variables, it was not tested experimentally.

11. COMPARISON RESULTS

Results are shown in Figs. 1 through 4, in terms of the fractional anaerobic volume of soil (FANVOL) plotted against time for soil layers 1, 7 and 15 corresponding to average depths of 0.8, 10.6 and 23.7 cm, respectively. The diffusion coefficient in the aggregates, and the rain intensity and duration were taken as 0.1272 $cm^2.d^{-1}$ and 9 $cm.d^{-1}$ and 3 hours, respectively.

Figure 1 serves as a so-called basic run in which input data for oxygen consumption rate and groundwater depth were taken 10 1 $O_2.m^{-2}$. 25 cm $depth^{-1}.d^{-1}$ and 100 cm, respectively. Input data used to produce Figs. 2, 3 and 4 have been changed as compared to those in Fig. 1 with respect to either oxygen consumption rate (26.7 1 $O_2.m^{-2}$. 25 cm $depth^{-1}.d^{-1}$), or spatial distribution of the respiratory activity, or groundwater depth (50 cm), respec-

tively. Before rain is introduced, about 0.05 day is needed to adjust FANVOL to its right initial value. It is seen that below a depth of 10 cm always some anaerobic microsites are present indicating the soil to be a potential source of denitrification. Further a rain of 11 mm has a pronounced effect on anaerobiosis even up to about 20 hours after it ceases.

A more detailed discussion is given by Leffelaar (1979).

12. LIMITS AND LIMITATIONS

- Maximum time step equals 10^{-4} day, caused by the small time constant of the macro oxygen diffusion process.
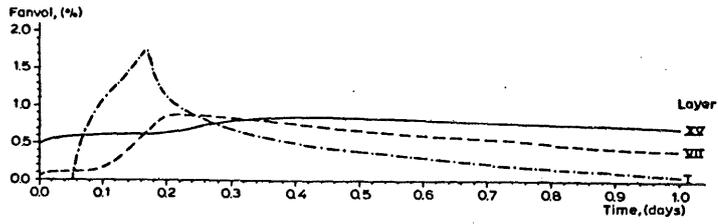
Fig. 1.
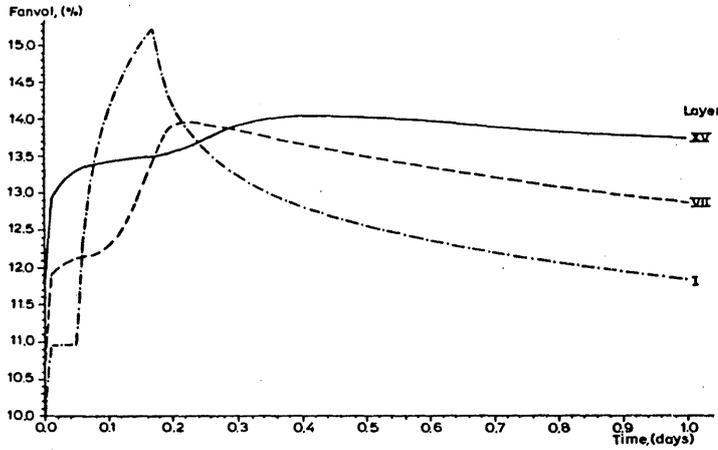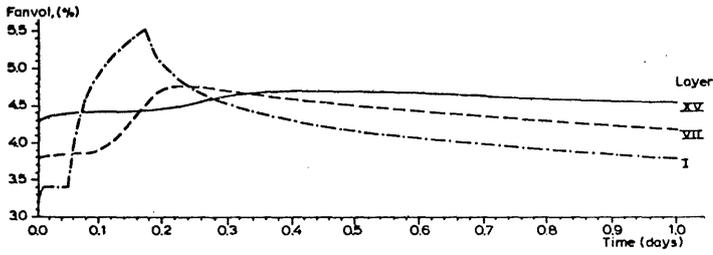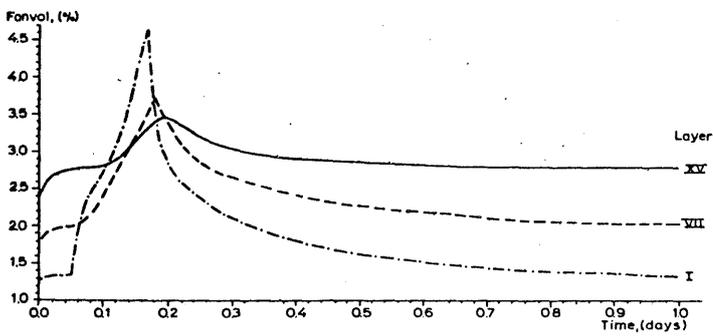

Fig. 2.

Fig. 3.

Fig. 4.

Figs. 1-4. FANVOL as a function of time for three layers. From top to bottom 1: basic program, run 1; 2: oxygen consumption 26.7 1 $O_2.m^{-2}$. 25 cm $depth^{-1}.d^{-1}$, run 2; 3: respiratory activity located in half the aggregates, run 3; 4: depth of groundwater table 50 cm, run 4. (Figs 1,2 and 4 from: Soil Science 128:110-120.Williams & Wilkins Co.Baltimore,USA)

- Space steps were taken as the height of a unit hexagonal packing. When the diameter of the equidimensional aggregates equal one cm this height is 1.633 cm.
- Minimum and maximum matric suctions are 1.017 and 2180 mbar, respectively, when the diameter of the equidimensional aggregates is one cm.
- Though the program may be used to investigate the relative importance of e.g. soil moisture characteristics or other aggregate diameters on anaerobiosis, such action would demand some recalculations of function tables.

13. COMPUTER

The model may be run on any computer that has a CSMP-III compiler available. These will be in general IBM machines (series 360 and 370) but for some other brands the same package is available (for instance DEC-10).

14. PROGRAM LANGUAGE

CSMP-III. However, the program may be rewritten in FORTRAN-4.

15. RUNNING TIME/COST

Costs were not registrated, but a run took about 120 sec CPU-time.

16. USERS

The model so far is only used by the developer.

17. DEVELOPER AND PRINCIPAL CONTACT

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18. REFERENCES

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