Reaction Kinetics for Modeling Non-Point Source Pollution of Nitrate with SWAT Model

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Water resources - vital statistics

- Rainfall: 4000 bcm/yr, translates into water resources (~48%), groundwater recharge (~11%).

- Water consumers - Agriculture (85%); Domestic (4%)

- Availability of water per capita (cu.m/ca/year)
  - World: 6700
  - North America: > 15,000
  - India: ~ 1200
Land per capita
1950’s: 0.89 ha
2000’s: 0.33 ha

Agriculture
Meeting requirements of food grains under limited land and water conditions
….asks for intensification (HYV, crop intensity)
Increase in irrigation and fertilizer use

Implications of intensification
### Impact of excessive use of nitrogenous fertilizers

<table>
<thead>
<tr>
<th>District</th>
<th>State</th>
<th>Nitrate (mg l(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mathura</td>
<td>Uttar Pradesh</td>
<td>279</td>
</tr>
<tr>
<td>Aligarh</td>
<td>Uttar Pradesh</td>
<td>270</td>
</tr>
<tr>
<td>Agra</td>
<td>Uttar Pradesh</td>
<td>240</td>
</tr>
<tr>
<td>Mahendragarh</td>
<td>Haryana</td>
<td>1310</td>
</tr>
<tr>
<td>Gurgaon</td>
<td>Haryana</td>
<td>722</td>
</tr>
<tr>
<td>Hisar</td>
<td>Haryana</td>
<td>419</td>
</tr>
<tr>
<td>Ambala</td>
<td>Haryana</td>
<td>419</td>
</tr>
<tr>
<td>Bhatinda</td>
<td>Punjab</td>
<td>567</td>
</tr>
<tr>
<td>Ludhiana</td>
<td>Punjab</td>
<td>265</td>
</tr>
<tr>
<td>Peddavoora</td>
<td>Andhra Pradesh</td>
<td>53</td>
</tr>
</tbody>
</table>

**Groundwater**

**Drinking water quality standard for nitrates: 45 mg l\(^{-1}\)**

**Surface water**

Data generated from its 480 river quality monitoring stations, mean nitrate values have increased from 0.4 mg l\(^{-1}\) in 1979 to 2.8 mg l\(^{-1}\) in 2000

Nitrate exceedence frequency i.e., %stations reporting nitrates exceeding the standard, has increased from 2% in 1979 to 10% in the year 2000


**Source** Kansal et al. (1992); CPCB, MINARS (1997)
Study area – Upper Yamuna river sub basin

Hypsometric curve

Scale: 1 cm = 14 km

District boundary
Catchment boundary
Streams
Precipitation distribution in the sub basin
<table>
<thead>
<tr>
<th>Subject area</th>
<th>Data basis</th>
<th>Source and map scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basic data</td>
<td>Boundaries of the river basin, administrative boundaries, stream networks</td>
<td>Survey of India (SoI); 1: 50 000</td>
</tr>
<tr>
<td>Climatic data</td>
<td>Mean monthly and daily precipitation, maximum and minimum temperature, solar radiation, wind speed, potential evaporation</td>
<td>Indian Meteorological Department (IMD)</td>
</tr>
<tr>
<td>Soil-physical data</td>
<td>Soil characteristics (% silt, sand, clay, rocks), field capacity, wilting point, hydraulic conductivity, depth to water table, properties for different soil layers varying with depth</td>
<td>National Bureau of Soil Survey and Land use planning (NBSS&amp; LUP); 1:250 000</td>
</tr>
<tr>
<td>Landuse data</td>
<td>Ground cover</td>
<td>SoI, Satellite Imageries, State Agricultural Board 1:50 000 and 1:250 000</td>
</tr>
<tr>
<td>Hydrogeological data and</td>
<td>Groundwater-bearing lithologic units, transmissivity, hydraulic conductivity, groundwater levels, fluctuations, hydrochemical data, water use (pumping and extraction)</td>
<td>Geological Survey of India (GSI); National Thematic Map Organization (NATMO), CGWB, SGWB, 1: 250 000</td>
</tr>
<tr>
<td>groundwater fluctuation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Topography data</td>
<td>Elevation contours</td>
<td>SoI; 1: 50 000</td>
</tr>
<tr>
<td>Gauge data</td>
<td>Daily river flows</td>
<td>Chander et al. (1984), Central Water Commission, Ministry of Water Resources</td>
</tr>
<tr>
<td>Crop and fertilizer data</td>
<td>Nitrogenous fertilizers use, crop yields and types of crops; gross and net cropped areas</td>
<td>Fertilizer Statistics, Fertilizer Association of India (FAI)</td>
</tr>
<tr>
<td>Water quality data</td>
<td>Surface water quality (Nitrate concentrations), ground water quality (nitrate concentrations)</td>
<td>Central Pollution Control Board (CPCB); State PCB, Station-wise</td>
</tr>
</tbody>
</table>
Results of SWAT

Daily stream flow (Damta upstream station)

Scatterplot of observed and simulated daily flows with the SWAT model (1976 to 1978, Damta upstream station)

Sub-basin | Damta upstream station
---|---
$R^2$ (daily) | 0.7248
Nash and Sutcliffe coefficient (daily) | 0.7104
Scatterplot of observed and simulated daily flows with the SWAT model (1976 to 1978, Lakhwar station)

Sub-basin | Lakhwar station
---|---
R² (daily) | 0.7717
Nash and Sutcliffe coefficient (daily) | 0.7417
Nitrate loads in surface water (Lakhwar)

**Daily flow (cumecs)**
- 0
- 10000
- 20000
- 30000
- 40000
- 50000
- 60000
- 70000

**Daily load (kg/day)**
- 0
- 1000
- 2000
- 3000
- 4000
- 5000
- 6000
- 7000
- 8000
- 9000
- 10000

**Date**
- 01/01/1976
- 02/20/1976
- 03/01/1976
- 04/20/1976
- 05/30/1976
- 07/19/1976
- 08/07/1976
- 09/27/1976
- 10/16/1976
- 11/04/1976
- 12/16/1976

**Daily nitrate load (kg/day)**
- 0
- 1000
- 2000
- 3000
- 4000
- 5000
- 6000
- 7000
- 8000
- 9000
- 10000

**Nitrate concentration at Lakhwar**
- 0
- 1
- 2
- 3
- 4
- 5
- 6

**Nitrate concentration (mg/l)**
- Maximum value for the year
- Minimum value for the year
- Mean daily value for the year
Nitrate loads in surface water (Giri at Yashwantnagar)

- - - - - - Daily flow (cusecs)  ● Daily nitrate load (kg/day)

Nitrate concentration at Yashwantnagar

Maximum value for the year  ■  Minimum value for the year  ● Mean daily value for the year
Summary of the results

The study has been successful in calibrating and validating the model consisting of the following components,

- Streamflow
- Groundwater levels
- Nitrates in surface water

- The simulated nitrate concentrations show a deviation from the observed values
- The model requires studying nitrate transformation processes in the unsaturated zone of the soil matrix since these have a direct bearing on nitrate transport in surface and groundwater
- Review of various models shows that Michaelis-Menten kinetics, a mixed-order kinetics, is well suited for simulating microbial action and growth under the influence of various environmental conditions and substrate concentration

This aspect has been studied further
Field tests for examining the kinetics

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Entisol</th>
<th>Anthrosol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Organic matter</td>
<td>g kg(^{-1})</td>
<td>2.9</td>
<td>11.8</td>
</tr>
<tr>
<td>Total N</td>
<td>g kg(^{-1})</td>
<td>0.2</td>
<td>0.8</td>
</tr>
<tr>
<td>NH(_4^+)</td>
<td>mg kg(^{-1})</td>
<td>8.2</td>
<td>2.3</td>
</tr>
<tr>
<td>NO(_3^-)</td>
<td>mg kg(^{-1})</td>
<td>11.5</td>
<td>9.2</td>
</tr>
<tr>
<td>pH</td>
<td></td>
<td>8.3</td>
<td>8.1</td>
</tr>
<tr>
<td>Water holding capacity</td>
<td>%</td>
<td>22.5</td>
<td>23</td>
</tr>
<tr>
<td>Density</td>
<td>g cm(^{-3})</td>
<td>1.1</td>
<td>1.2</td>
</tr>
</tbody>
</table>

*Particle size distribution*

<table>
<thead>
<tr>
<th></th>
<th>%</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand (2–0.02 mm)</td>
<td></td>
<td>68.9</td>
<td>27.5</td>
</tr>
<tr>
<td>Silt (0.02–0.002 mm)</td>
<td></td>
<td>24.6</td>
<td>49.0</td>
</tr>
<tr>
<td>Clay (&lt;0.002 mm)</td>
<td></td>
<td>6.5</td>
<td>23.5</td>
</tr>
</tbody>
</table>
Simulation results and comparison of kinetics

Simulation of nitrification using published data

Simulation of nitrification in Anthrosols

Experimental station | $R^2$ | Nash and Sutcliffe
--- | --- | ---
SWAT (Entisol) | 0.75 | 0.83
Michaelis-Menten (Entisol) | 0.98 | 0.98
SWAT (Anthrosol) | 0.85 | 0.90
Michaelis-Menten (Anthrosol) | 0.96 | 0.98
Simulation results on influence of soil moisture on denitrification

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**Experimental station** | **R²** | **Nash and Sutcliffe**
--- | --- | ---
SWAT, Case 1; (Case 2) | 0.93; (does not simulate) | 0.86; (does not simulate)
Michaelis-Menten, Case 1; (Case 2) | 0.97; (0.97) | 0.96; (0.96)
Conclusions

- Nitrate transport to surface water and groundwater aquifers takes place under the influence of the runoff components of the land phase of the hydrological cycle.

- The kinetics of nitrate transformation processes namely, nitrification and denitrification, in the land phase of the hydrological cycle determines the transformation and release of nitrates in surface and groundwater aquifers.

- The transformation of nitrates is governed by bacteriological action, which can be best represented by mixed order kinetics, i.e., Michaelis Menten Kinetics.

- The comparison of the existing first-order kinetics with the proposed Michaelis-Menten mixed order kinetics indicates that Michaelis-Menten mixed order kinetics represents the nitrate transformation processes better.
Limitations of the study

- A longer length of record would have been desirable for calibration and validation of various components of the integrated model.

- Nitrate concentration data for surface water was limited.

- Fertilizer application data was limited.
Future scope of research

The Michaelis-Menten mixed order kinetics has been successfully tested using published experimental datasets. Incorporating it in the SWAT model itself and simulating nitrate transformations could be done in the future.
thank you