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

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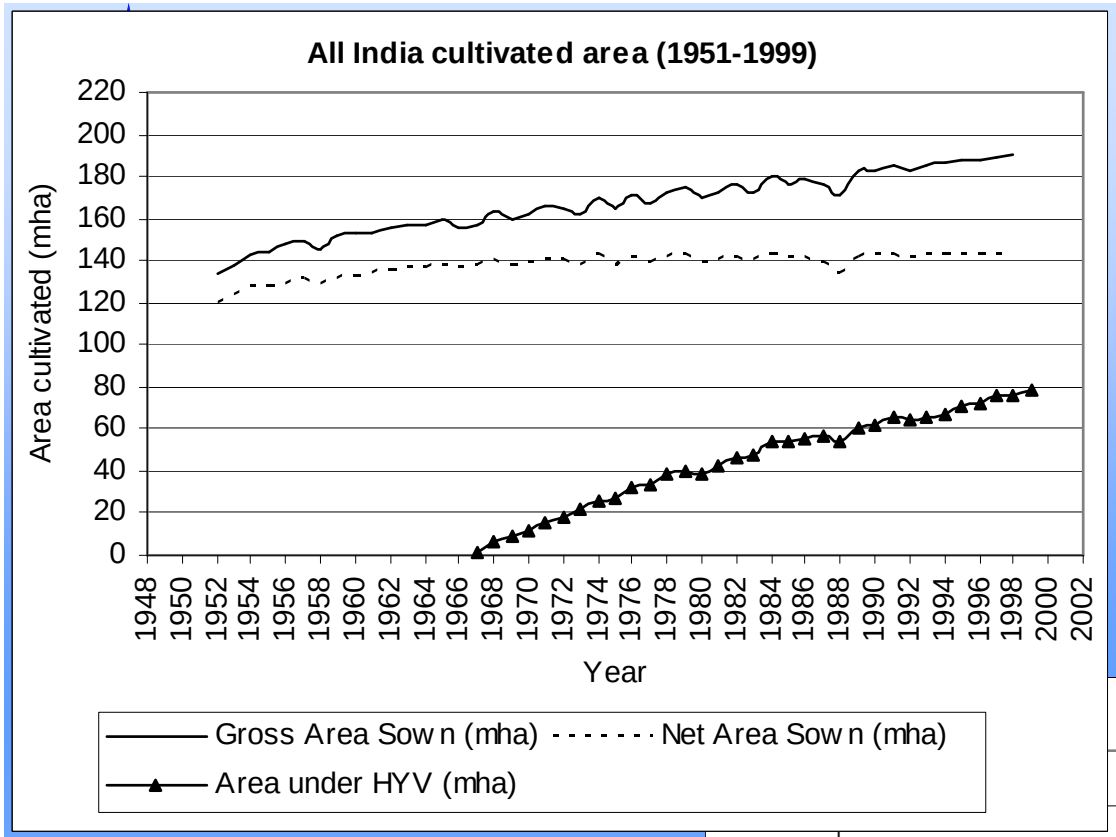
Water resources - vital statistics

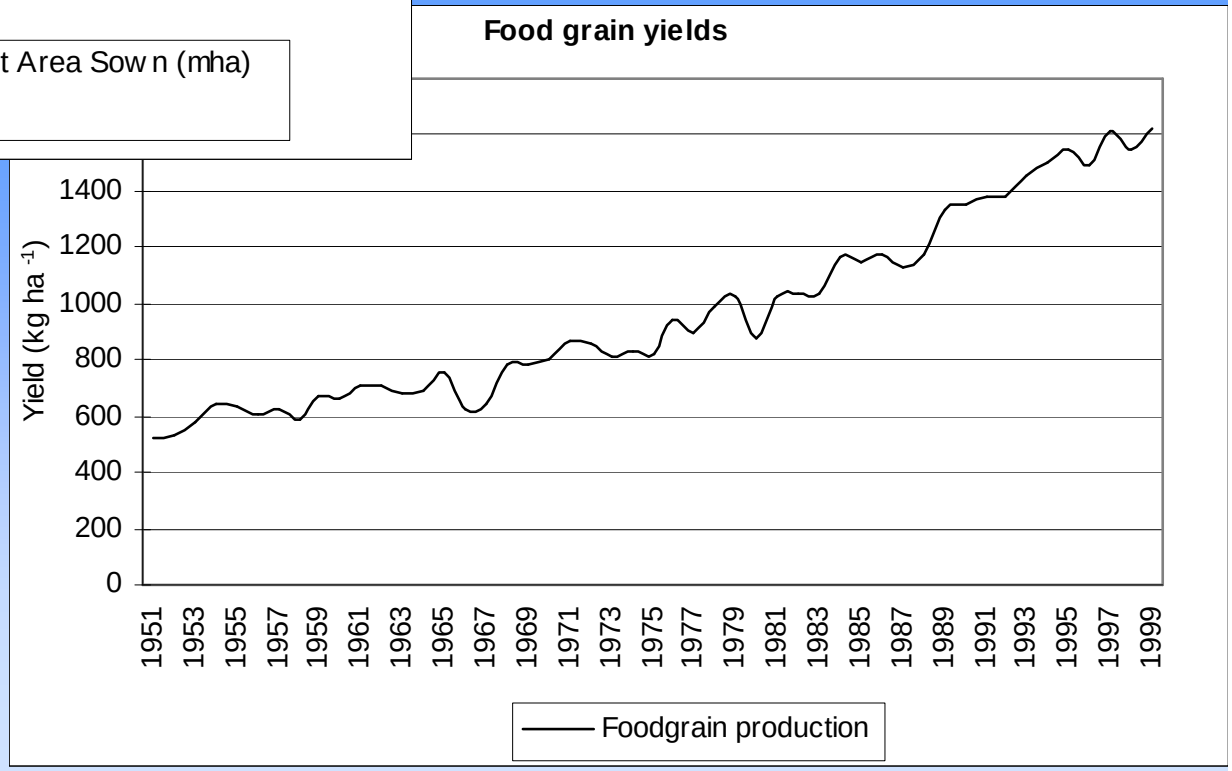
- Rainfall: 4000 bcm/yr, translates into water resources (~48%), groundwater recharge (~ 11%).
- Water consumers - Agriculture (85%); Domestic (4%)
- Availability of water per capita (cu.m/ca/year)
  - World: 6700
  - North America : > 15,000
  - India : ~ 1200

Agriculture

Meeting requirements of food grains under limited land and water conditions

….asks for *intensification* (HYV, crop intensity)

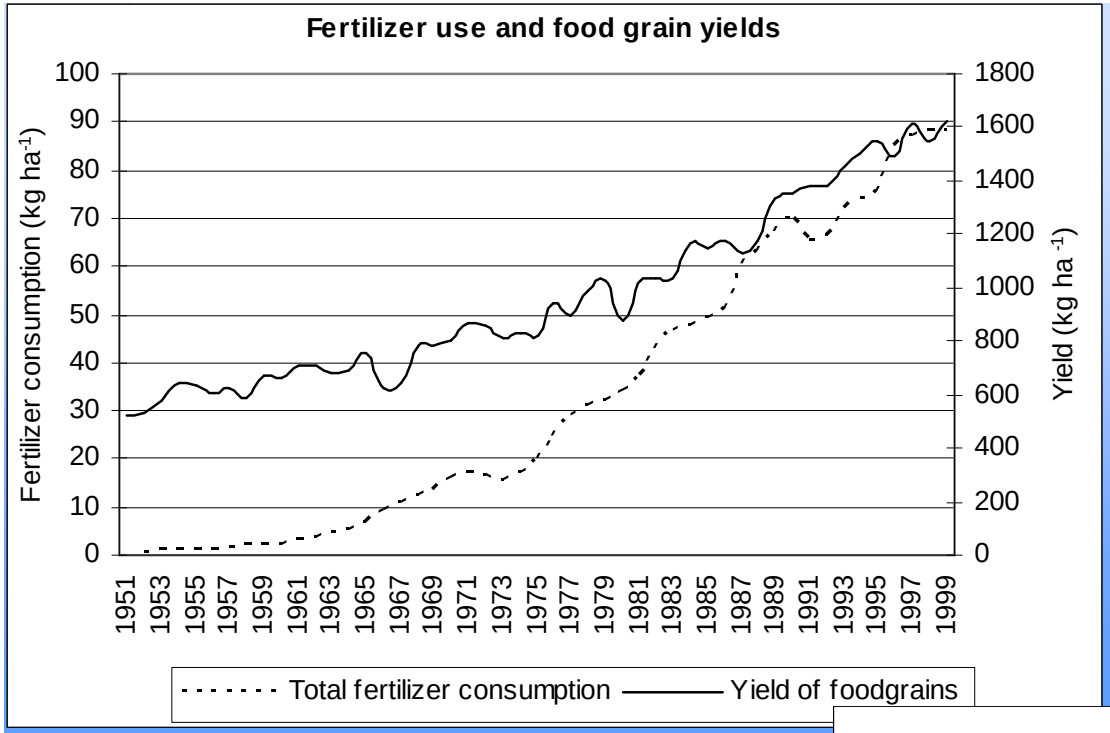




Land per capita

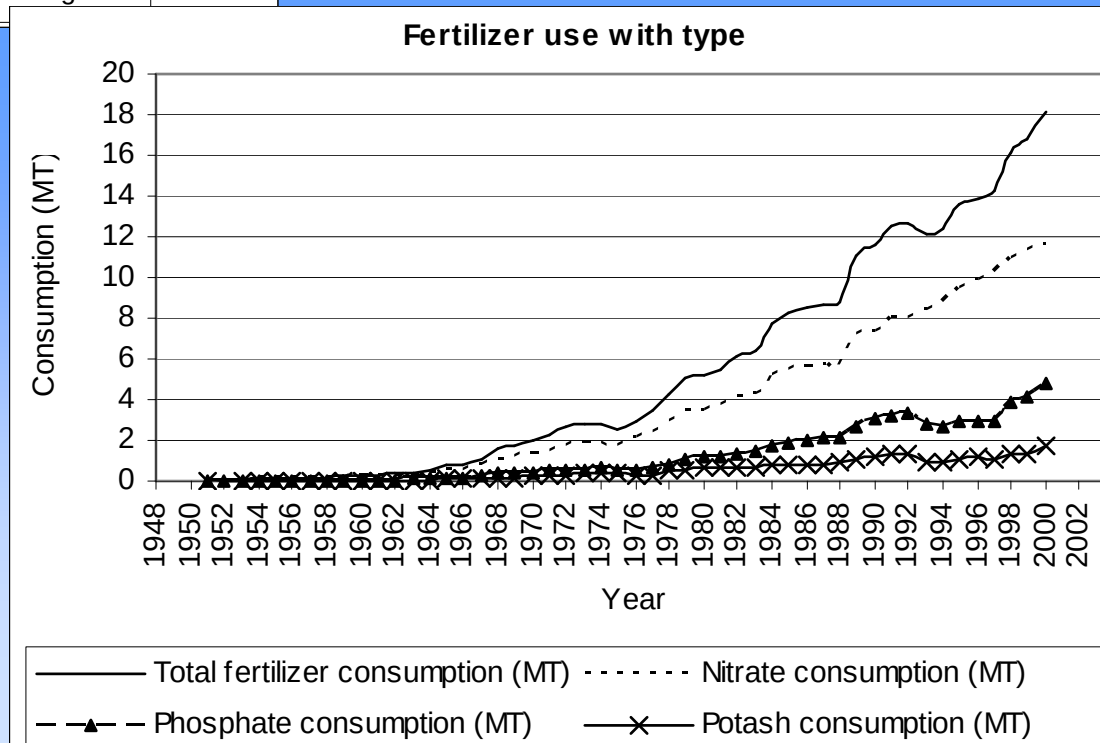
1950's: 0.89 ha

2000's: 0.33 ha



Implications of intensification

Increase in irrigation and fertilizer use



Impact of excessive use of nitrogenous fertilizers

Groundwater

Drinking water quality standard for nitrates: 45 mg l^{-1}

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

Source Kansal et al. (1992); CPCB, MINARS (1997)

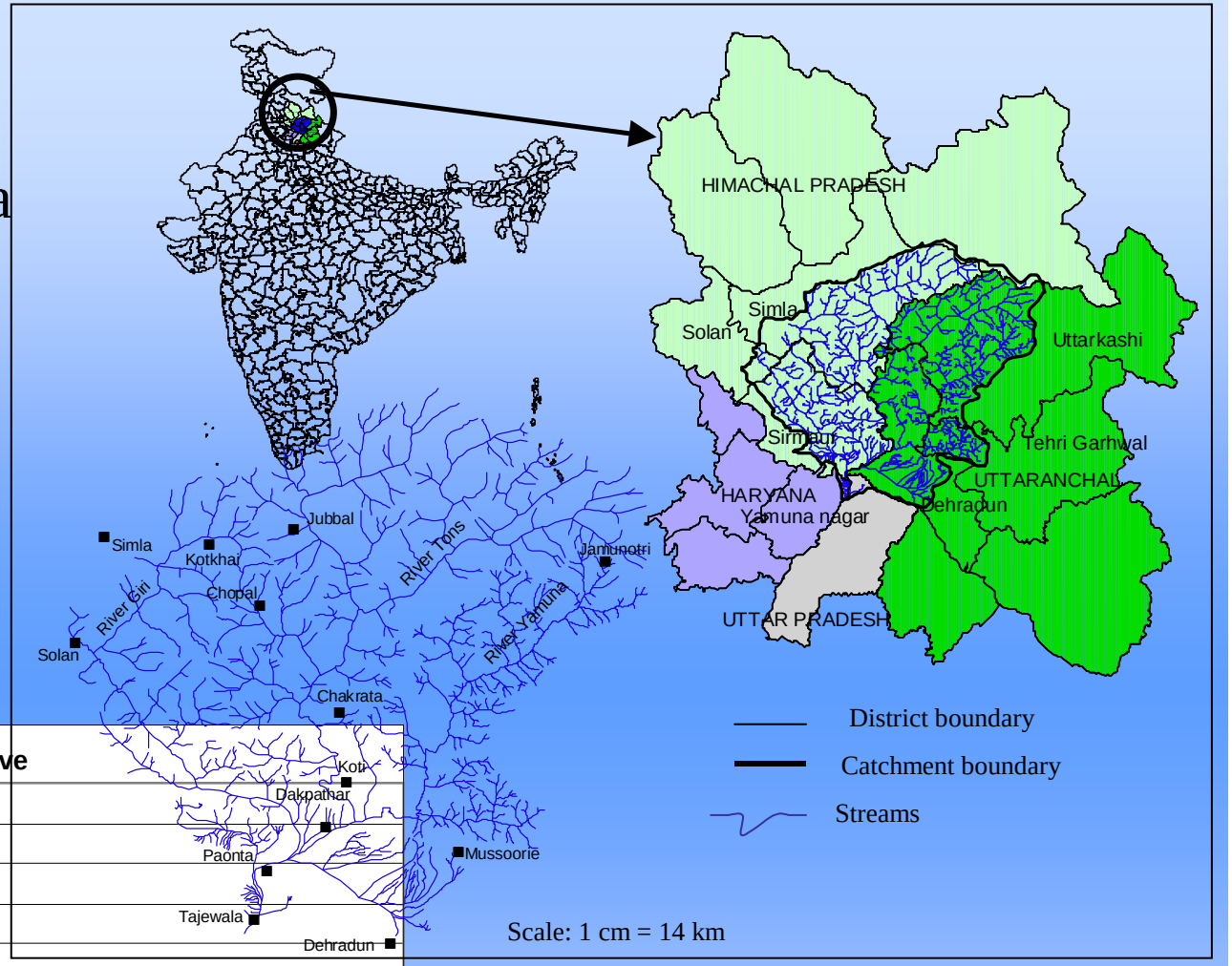
Surface water

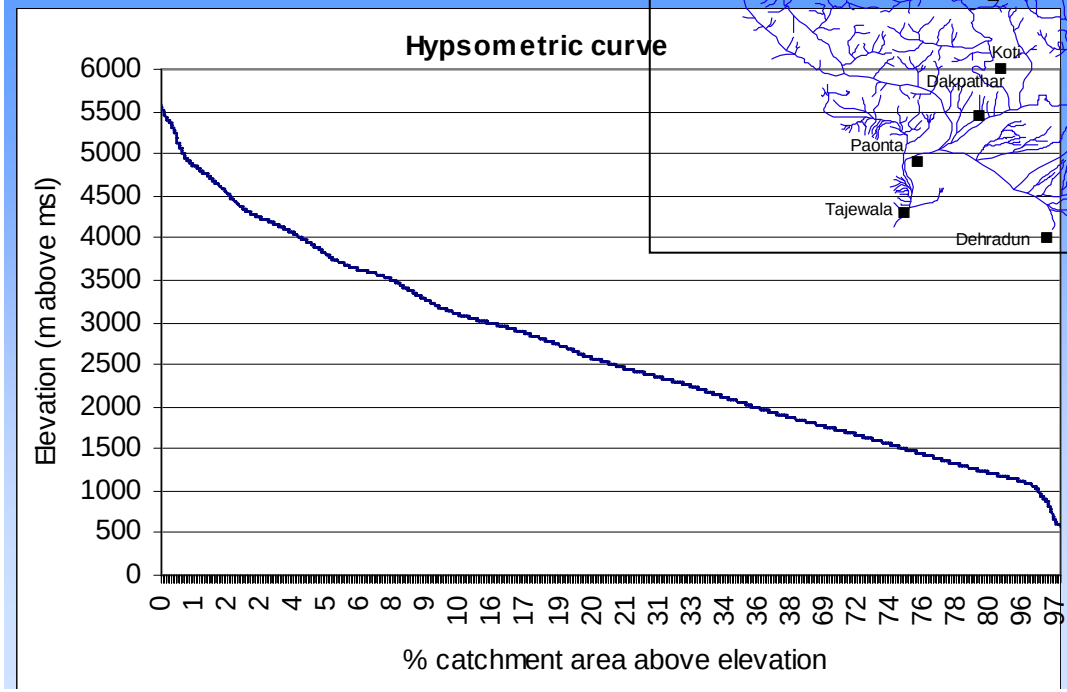
Data generated from its 480 river quality monitoring stations, mean nitrate values have increased from 0.4 mg l^{-1} in 1979 to 2.8 mg l^{-1} in 2000

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

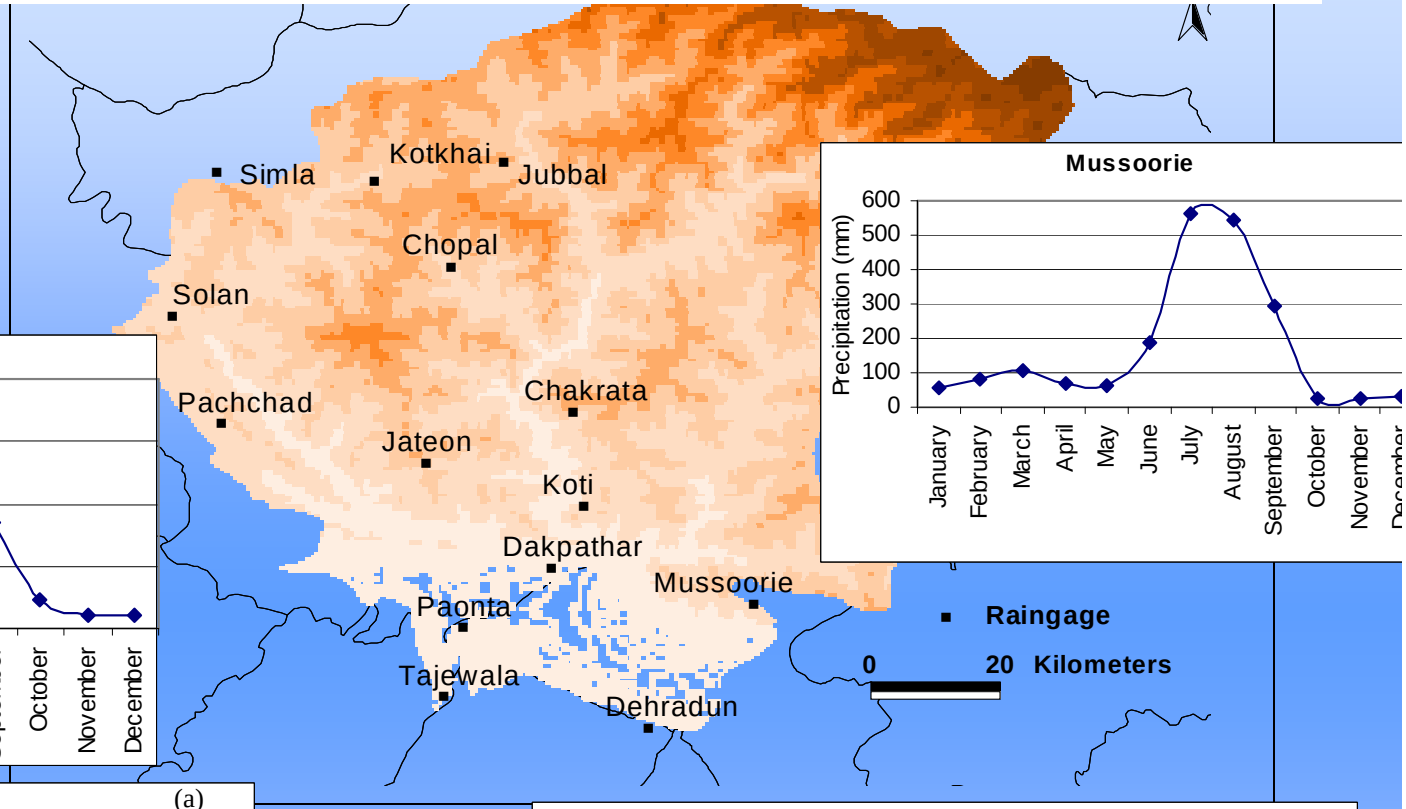
(Source: Analysed from datasets published by CPCB, MINARS Series 1979–2001).

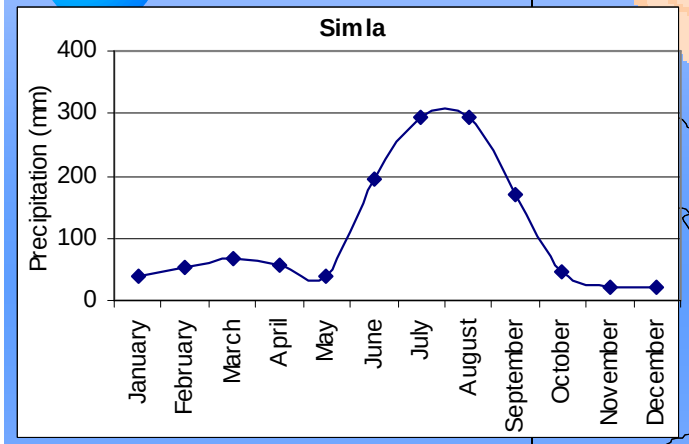
Study area – Upper Yamuna river sub basin

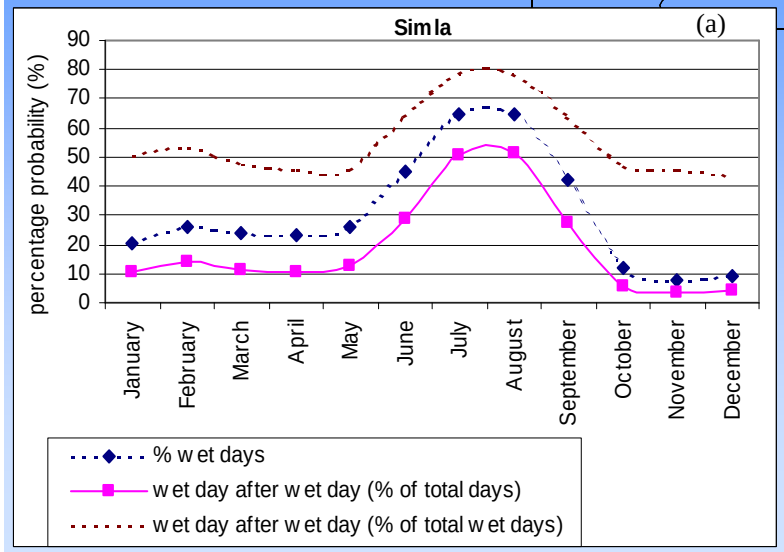


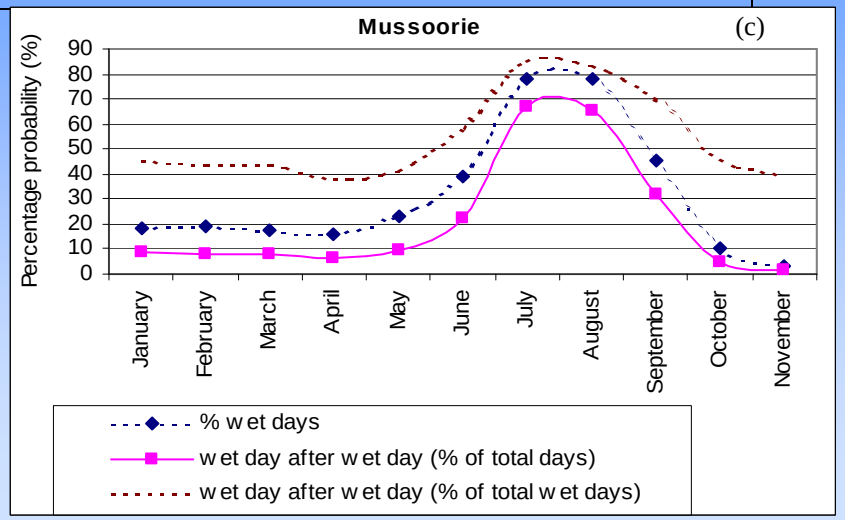


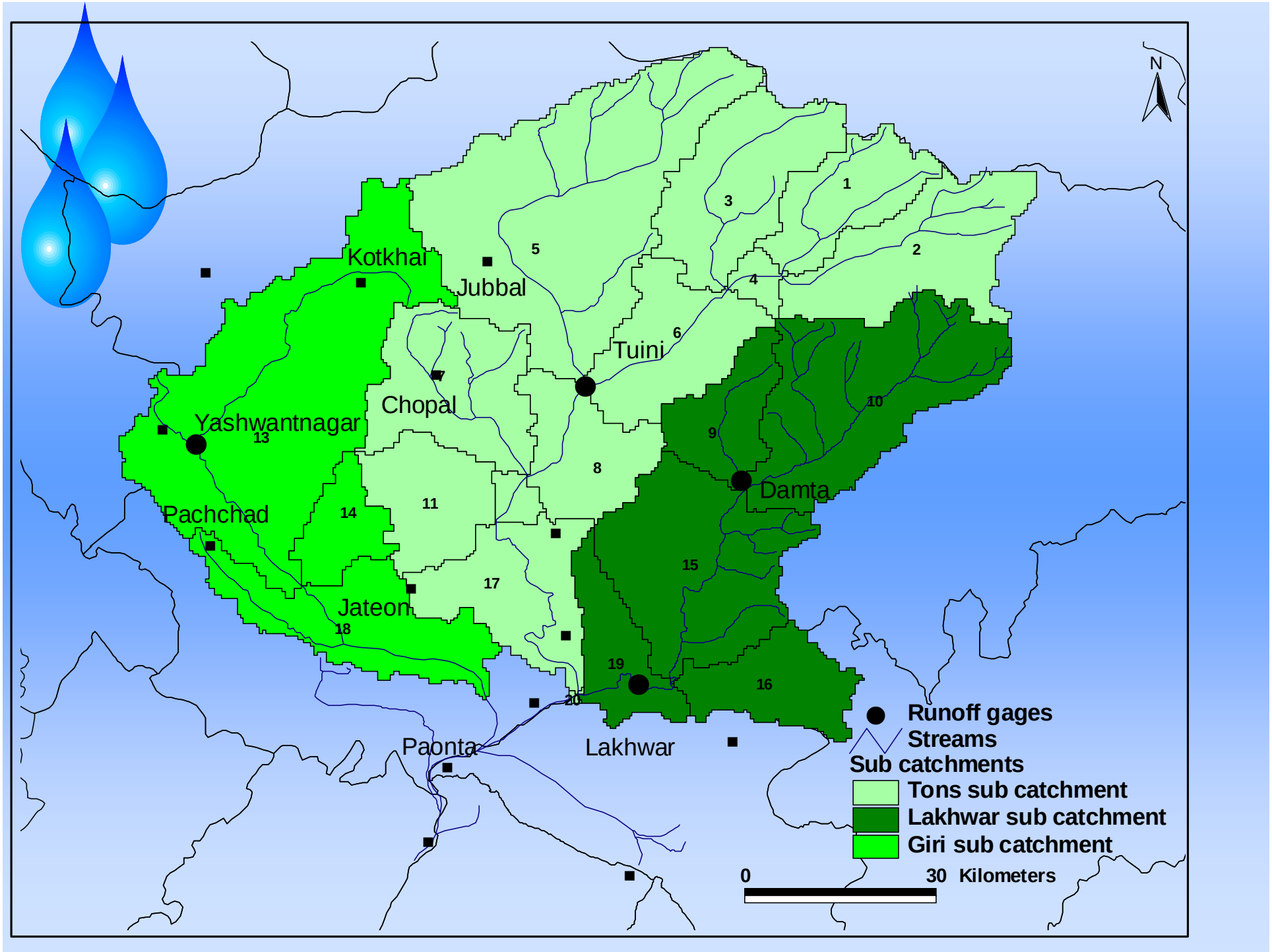
Precipitation distribution in the sub basin





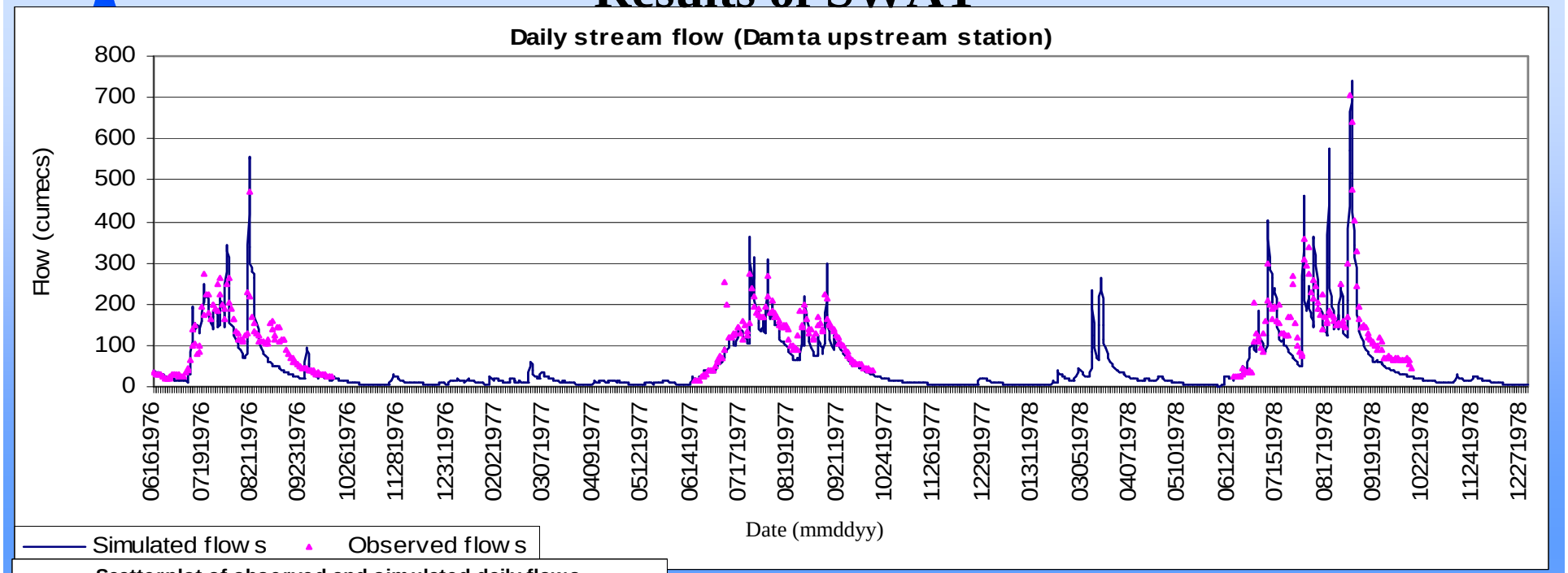


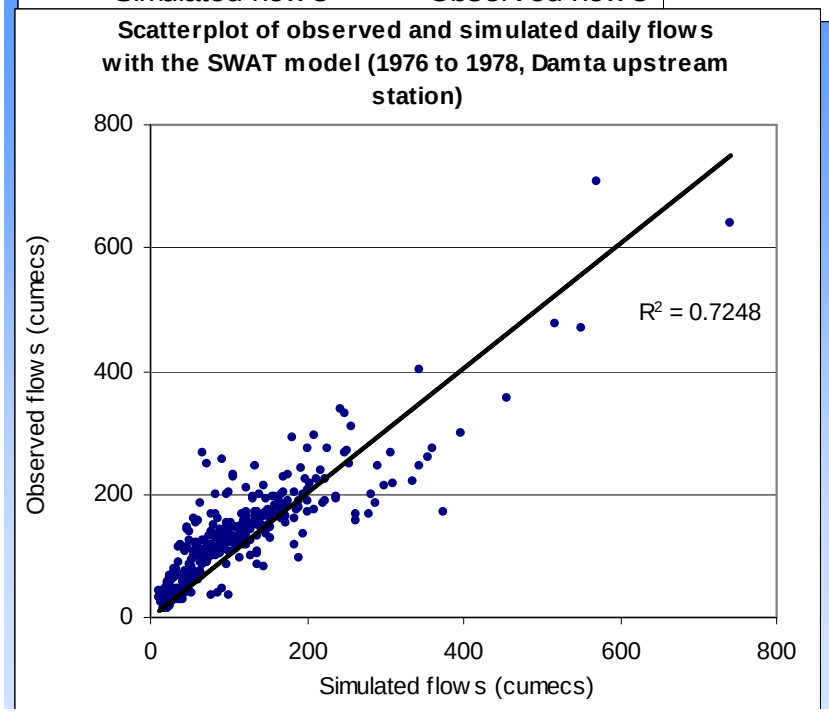



N
Kotkhai
Jubbal
Tuini
Chopal
Yashwantnagar
Pachchad
Jateon
Damta
Paonta
Lakhwar
1
2
3
4
5
6
7
8
9
10
11
13
14
15
16
17
18
19
20
Runoff gages
Streams
Sub catchments
Tons sub catchment
Lakhwar sub catchment
Giri sub catchment
0
30 Kilometers

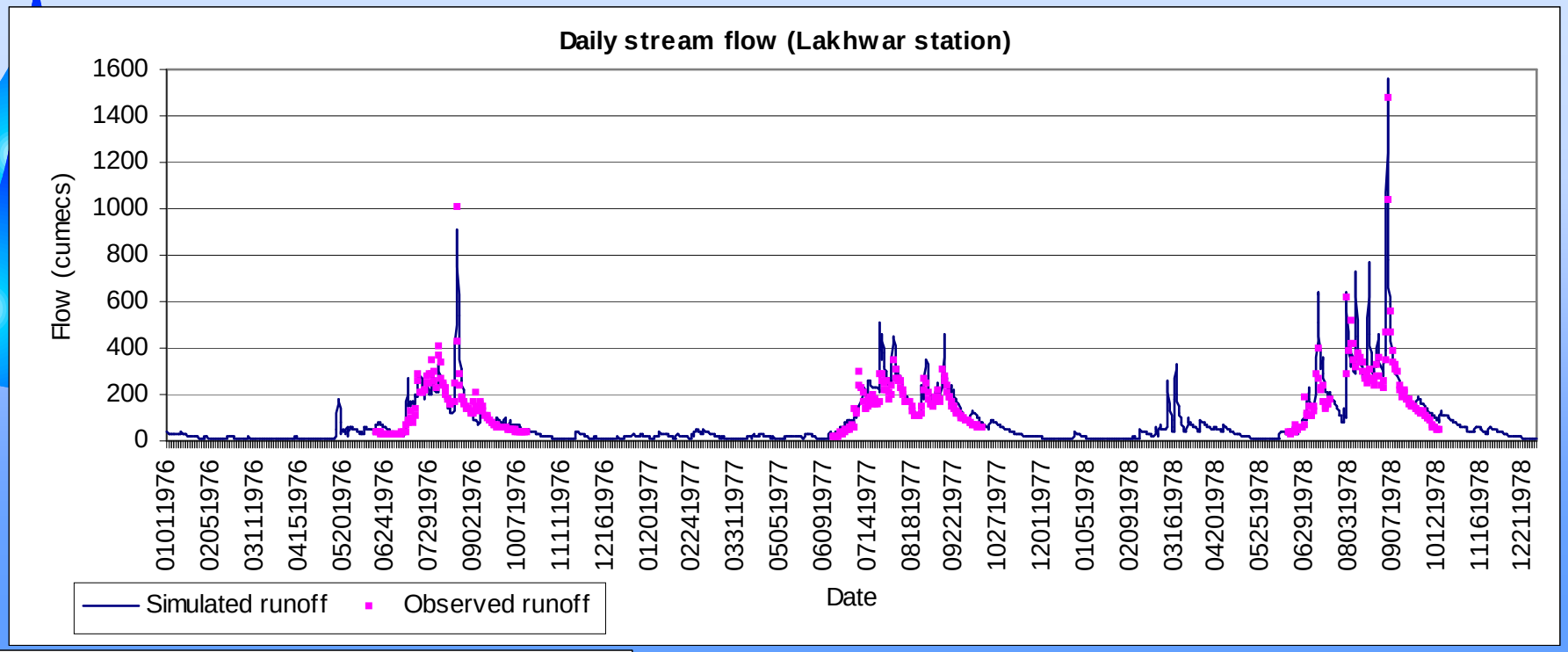
Subject area	Data basis	Source and map scale
Basic data	Boundaries of the river basin, administrative boundaries, stream networks	Survey of India (SoI); 1: 50 000
Climatic data	Mean monthly and daily precipitation, maximum and minimum temperature, solar radiation, wind speed, potential evaporation	Indian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

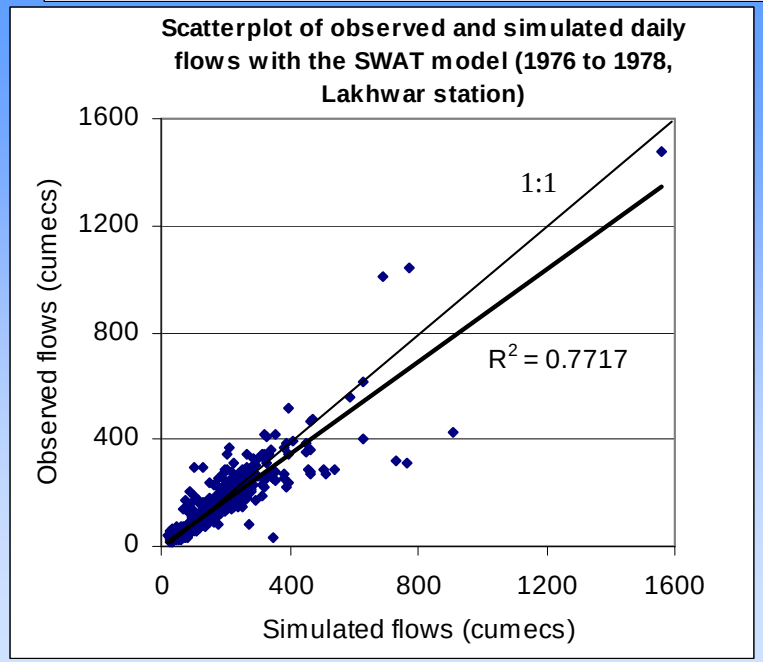
Results of SWAT



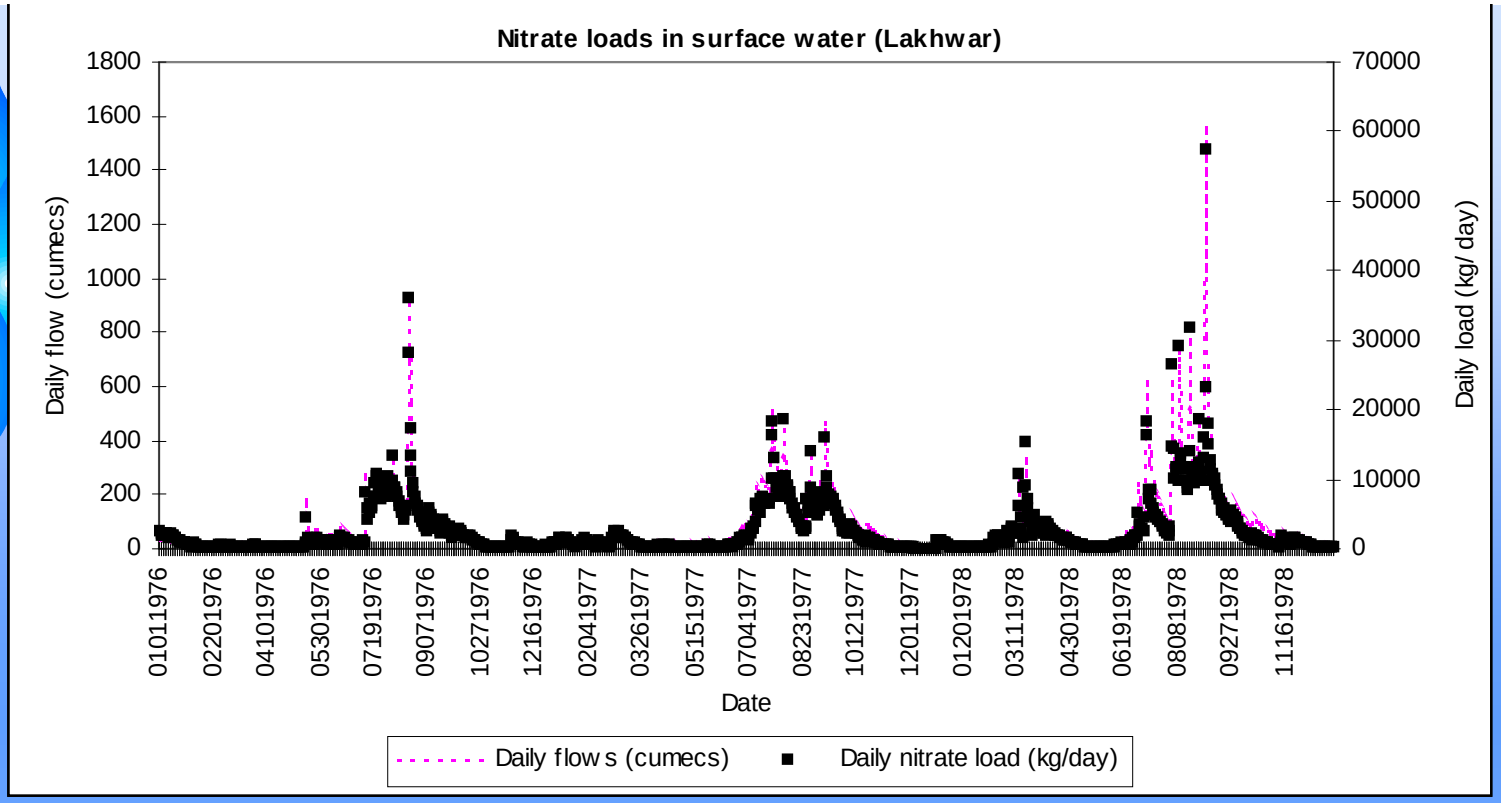


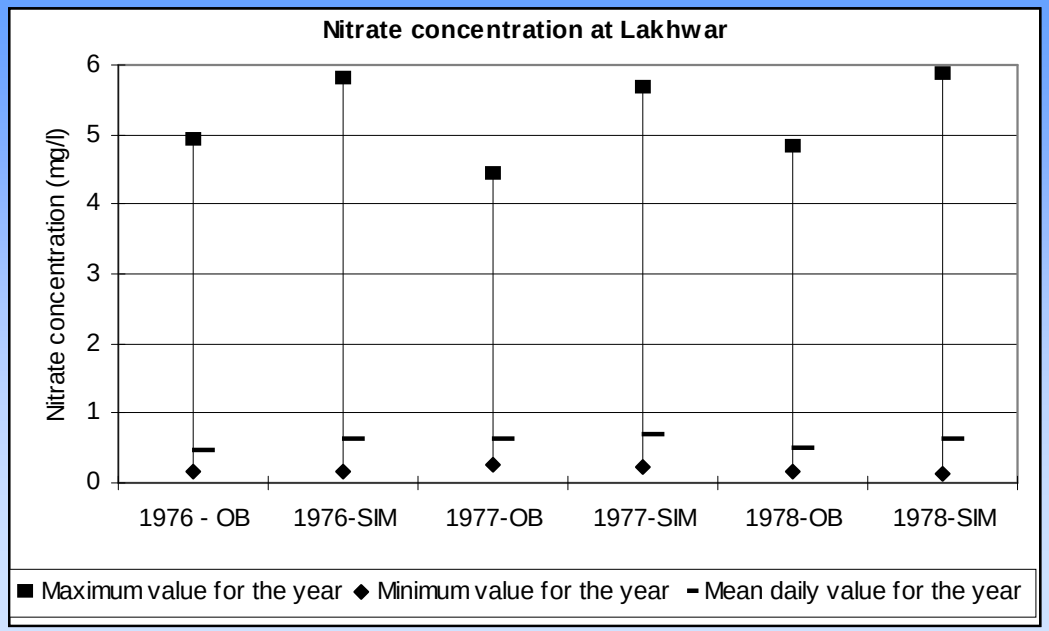
Sub-basin	Damta upstream station
R^2 (daily)	0.7248
Nash and Sutcliffe coefficient (daily)	0.7104

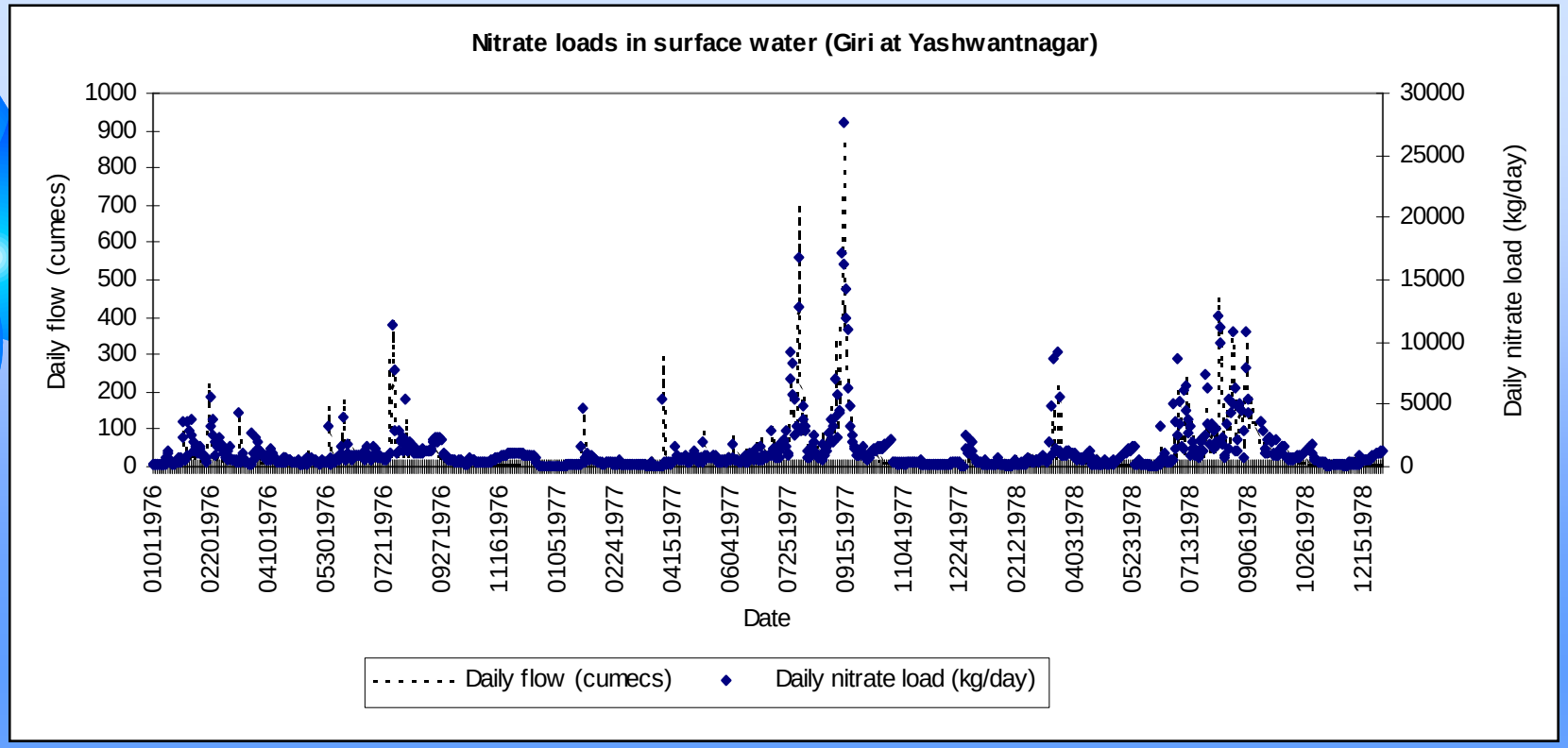


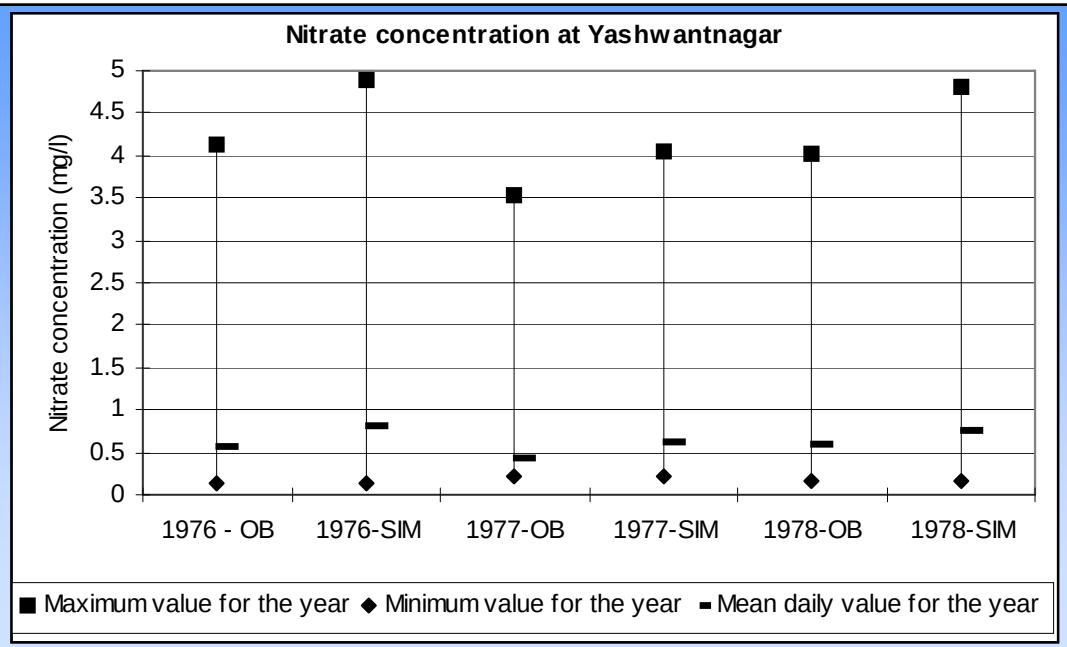


Sub-basin	Lakhwar station
R^2 (daily)	0.7717
Nash and Sutcliffe coefficient (daily)	0.7417


Nitrate loads in surface water (Lakhwar)
Daily flow (cumecs)
Daily load (kg/ day)
Date
1800
1600
1400
1200
1000
800
600
400
200
0
70000
60000
50000
40000
30000
20000
10000
0
01011976
02201976
04101976
05301976
07191976
09071976
10271976
12161976
02041977
03261977
05151977
07041977
08231977
10121977
12011977
01201978
03111978
04301978
06191978
08081978
09271978
11161978
Daily flow s (cumecs)
Daily nitrate load (kg/day)


Nitrate concentration at Lakhwar
Nitrate concentration (mg/l)
6
5
4
3
2
1
0
1976 - OB
1976-SIM
1977-OB
1977-SIM
1978-OB
1978-SIM
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 (cumecs)
Daily nitrate load (kg/day)
1000
900
800
700
600
500
400
300
200
100
0
30000
25000
20000
15000
10000
5000
0
01011976
02201976
04101976
05301976
07211976
09271976
11161976
01051977
02241977
04151977
06041977
07251977
09151977
11041977
12241977
02121978
04031978
05231978
07131978
09061978
10261978
12151978
Date
Daily flow (cumecs)
Daily nitrate load (kg/day)


Nitrate concentration at Yashwantnagar
Nitrate concentration (mg/l)
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1976 - OB
1976-SIM
1977-OB
1977-SIM
1978-OB
1978-SIM
Maximum value for the year
Minimum value for the year
Mean daily value for the year

Summary of the results

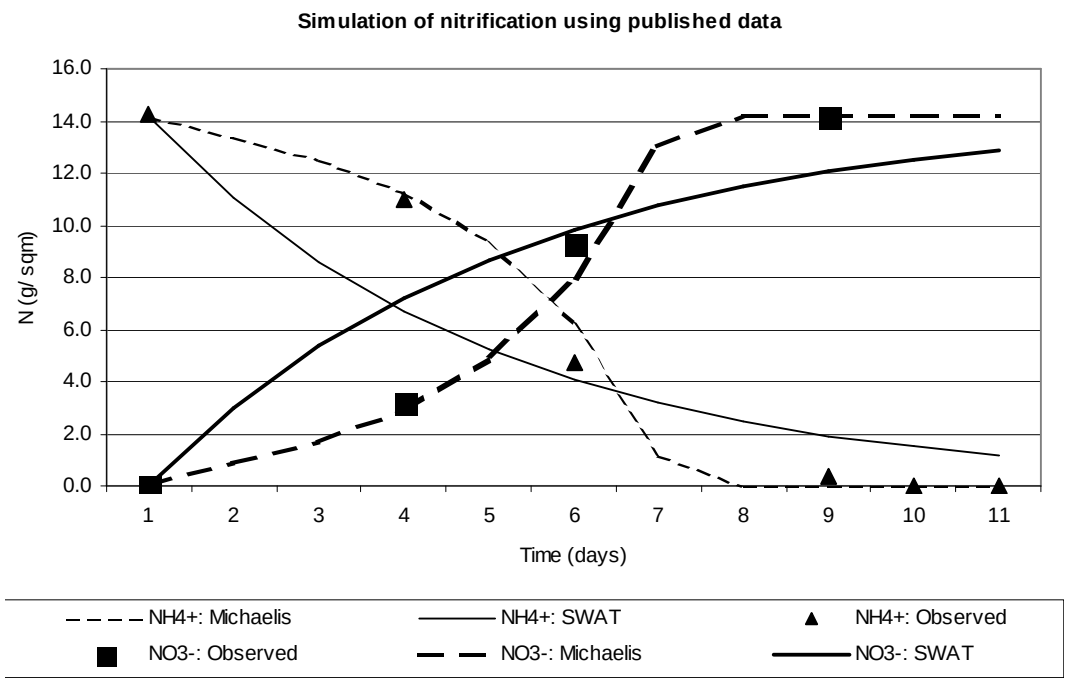
- The study has been successful in calibrating and validating the model consisting of the following components,
  - Streamflow
  - Groundwater levels
  - Nitrates in surface water
- The simulated nitrate concentrations show a deviation from the observed values
- The model requires studying nitrate transformation 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

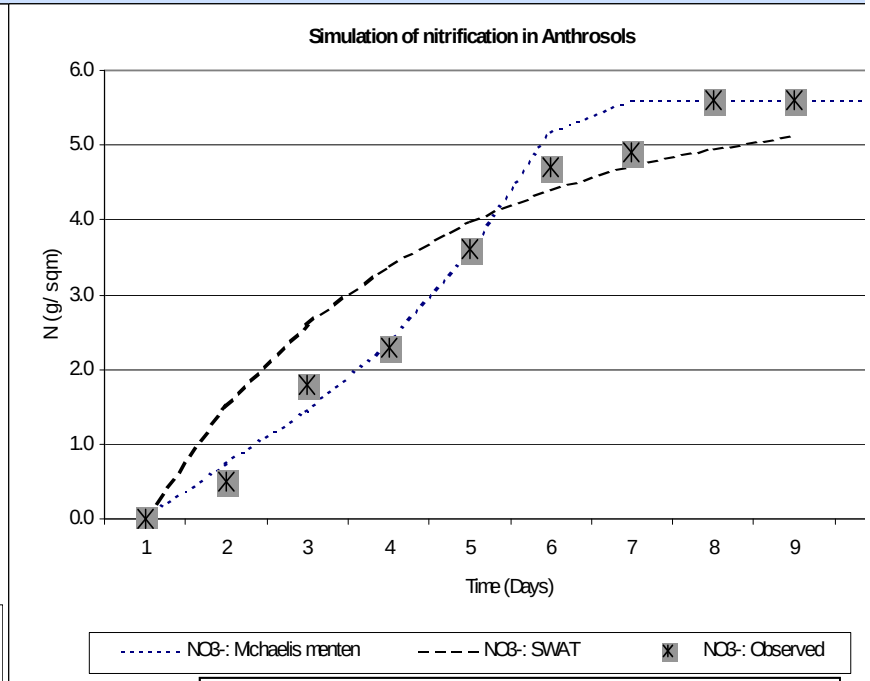
This aspect has been studied further

Field tests for examining the kinetics

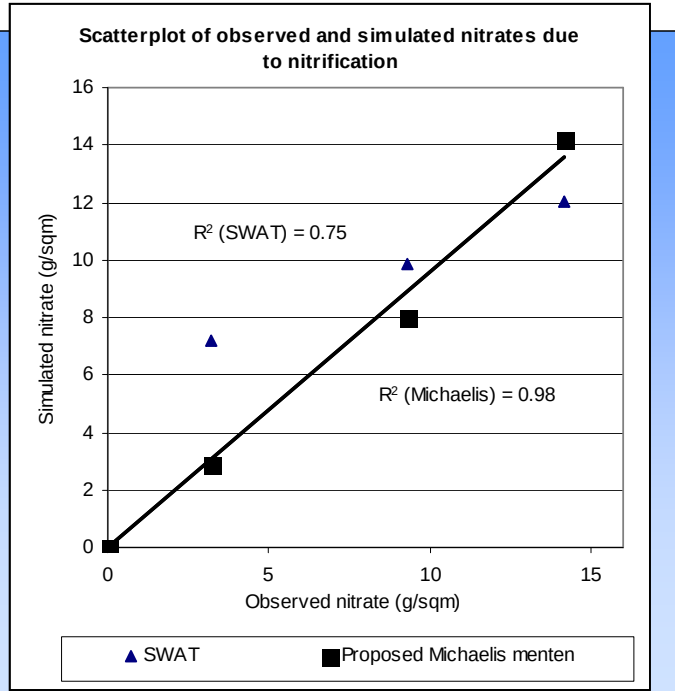
Parameter	Unit	Entisol	Anthrosol
Organic matter	g kg^{-1}	2.9	11.8
Total N	g kg^{-1}	0.2	0.8
NH_4+	mg kg^{-1}	8.2	2.3
NO_3-	mg kg^{-1}	11.5	9.2
pH		8.3	8.1
Water holding capacity	%	22.5	23
Density	g cm^{-3}	1.1	1.2
Particle size distribution			
Sand (2–0.02 mm)	%	68.9	27.5
Silt (0.02–0.002 mm)	%	24.6	49.0
Clay (<0.002 mm)	%	6.5	23.5

Simulation results and comparison of kinetics

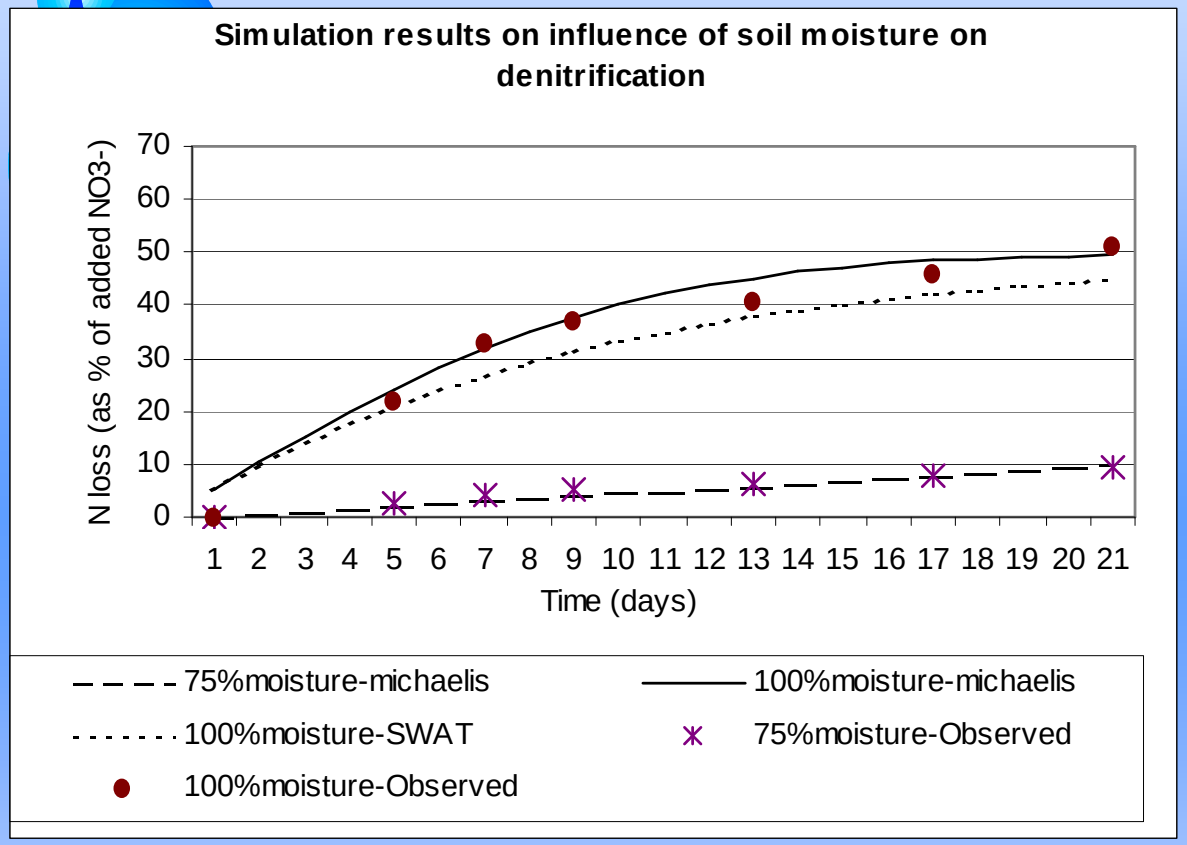


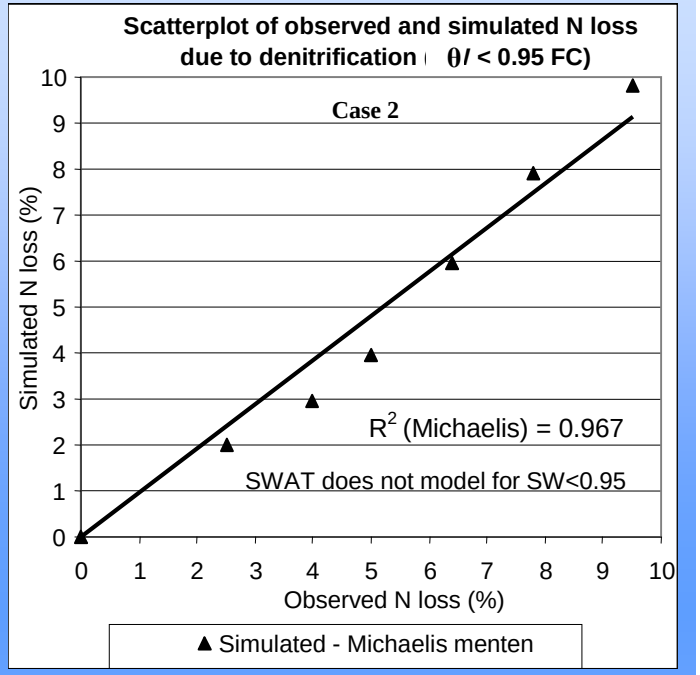


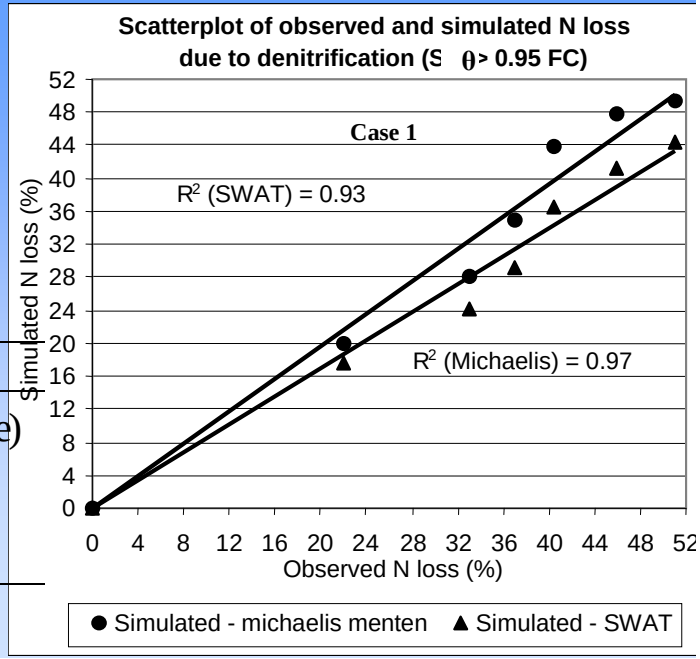
Experimental station	R^2	Nash and Sutcliffe
SWAT (Entisol)	0.75	0.83
Michaelis-Menten (Entisol)	0.98	0.98
SWAT (Anthrosol)	0.85	0.90
Michaelis-Menten (Anthrosol)	0.96	0.98



…..simulation results and comparison of kinetics







Experimental station	R^2	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