Naturalista sicil., S. IV, XXI (1-2), 1997, pp. 93-107

PAOLO MADONIA, ROCCO FAVARA & MARIANO VALENZA

COMPUTER MODELING OF ISOTOPIC COMPOSITION OF PRECIPITATION: A GIS BASED METHOD

SUMMARY

The abundance of stable isotopes have been often used as natural tracer, especially to study the evolution of surface and underground water. Starting from isotopic data, collected in pluviometric stations, is then necessary, if quantitative or semi-quantitative evaluations must be performed, to develop procedures by which punctual data can be extended to a three-dimensional surface. This paper presents the preliminary results of the development of an automatic isotopic modeling method of hydrological systems, based on Geographical Informative System (GIS) ARC/INFO.

RIASSUNTO

Modellistica automatizzata della composizione isotopica delle precipitazioni atmosferiche: un approccio basato sui Sistemi Informativi Geografici. Le abbondanze degli isotopi stabili sono spesso usate come traccianti naturali, specialmente per ciò che concerne lo studio delle acque superficiali e sotterranee. Partendo da dati di composizione isotopica acquisiti in stazioni pluviometriche, se devono essere eseguite elaborazioni quantitative o semi-quantitative, risulta necessario sviluppare procedure in base alle quali i dati puntuali possono essere estesi a superfici tridimensionali. Il presente lavoro illustra i risultati preliminari riguardanti lo sviluppo di una procedura automatica, basata sui Sistemi Informativi Geografici ed in particolare sul noto ARC/INFO, che consente di valutare la composizione isotopica media annua delle precipitazioni atmosferiche in una data area. Come area campione per la taratura del metodo è stato scelto il Parco Naturale Regionale delle Madonie.

INTRODUCTION

The abundance of stable isotopes have been often used as natural tracer, especially to study the evolution of surface and underground waters. The isotopic signature of natural waters, in terms of $\delta^{18}O$ and δD (GONFIANTINI, 1978), constitutes important information in understand the complex relationships between rain, water reservoirs and springs in hydrogeologic circuits.

This paper presents the preliminary results of the development of an automatic isotopic modeling method of hydrological systems. A logical approach for an automatic precipitation isotopic modeling methodology, based on Geographical Informative System (GIS) ARC/INFO, is discussed; the method has been applied in the karst area of Madonie Mounts, Northern Sicily, Italy.

The GIS software chosen for the implementation of the methodology is ARC/INFO (release 6.0 under UNIX operating system) installed on a SUN Sparcstation 2. The ARC/INFO data model is composed of geographic data sets; the are two types of spatial information, locational and descriptive. Attribute data for each geographic feature are stored in a set of tables linked to the corresponding spatial data, so that both sets of information are always available. Many spatial features are defined topologically in a coverage. There are two common methods used for surface representation in ARC/INFO: Tins and Lattices.

A Tin is a set of adjacent, non overlapping triangles computed from irregular spaced points with xyz values. The Tin triangulation method satisfies the DELAUNAY criteria (ESRI, 1991): this means that a circle drawn through the three nodes of a triangle will not contain other points.

A Lattice is the surface interpretation of a grid of equally spaced sample points, referenced to a common origin and a constant sampling distance in the x and y directions. In a Lattice each mes point represents a value on the surface only at the center of the grid cell; it does not imply an area of constant value. The number of sample points in x and y direction defines the lattice resolution. The distance between sample points is the same in both x and y directions.

VARIABLES AFFECTING ISOTOPIC COMPOSITION OF PRECIPITATION

Osygen isotopic composition of precipitation is influenced by may factors, which depend upon either the kinetic and thermodynamics of the condensation processes by which rain, hail and snow are generated, or the interaction between these condensed particles, atmosphere and orographic structures.

Oxygen isotopic composition, expressed in the well known δ notation (GONFIANTINI, 1978), can be used as a tracer to determinate the relationships between watersheds and springs, by the comparison of the average $\delta^{18}O$ values of precipitation in a supposed alimentation area and in the related springs. Starting with isotopic data, collected in pluviometric stations, it is the necessary, if quantitative or semi-quantitative evaluations must be performed, to develop procedures by which punctual data can be extended to a three-dimensional surface like a watershed.

The very complex isotopic fractionation processes occurring during the water cycle can be simplified and described by a relatively small number of variables, according to the precision level needed in the hydrological application.

Data from I.A.E.A. network (YURTSEVER & GAT, 1981), have been compared with a series of geographical and metereological parameters by multiple linear regression analysises (Table I).

Tab. I

Results of multiple linear regression analyses for weighted mean of $\delta^{18}O$; T is average monthly temperature in °C, P is average monthly rainfall amount in mm, L is latitude in degrees, A is altitude in m a.s.l.

Independent variables	Regression coefficients	(± δ)
T, P, L, A,	0.797	2.82
T, P, L	0.795	2.82
T, P	0.785	2.86
T	0.785	2.84

In discussing the result, the Authors notice that on a global scale only temperature seem to play a fundamental role in determing isotopic composition, whereas on a regional scale factors such as amount of precipitation and evaporation may assume great importance.

By a critical revies of the data discussed by YURTSEVER & GAT, three main factors should be considered in a watershed/springs modeling: distance from the sea (better known as 'Continentality effect'), amount of precipitation and ground level temperature. Typical values for each of these variables (YURTSEVER & GAT, 1981) are reported in Table II.

Tab. II

Variables affecting isotopic composition of precipitations on a regional scale (after YURTSEVER & GAT, 1981)

Effect definition	Unit of measure	Typical values
Continentality	δ/Km	0.75 - 3
Ground level temperature	δ/°	0.34
Precipitation amount	δ/100 mm	0.84 - 1.5

The selected parameters constitute the base with which all modeling procedures described in the following chapters have been developed.

Description of the methodology

The ideal precision limit of an automatic modeling procedure can be considered equal to the experimental error in laboratory determination of $\delta^{18}O$, that means about 0.3 δ‰ (standard of the IAEA Isotope Hydrology Laboratory).

Estimation errors of the modeling procedures are the results of the sum of two different errors:

1) Estimation errors affecting interpolation methods from punctual sampling points to three-dimensional distributions;

2) Estimation errors of statistically derived formulas linking isotopic composition to meteorological and geographical factors. The amount of errors depends on the number **n** of sampling points involved in the model; **n** may theoretically variates from ∞ to **1**. An infinite number of points will ensure the model perfectly responds to the real world. Considering only one point it is possible to develop a model but it is impossible to check it; a model generated from only one measured value needs at least one other sampling points to calculate residuals between measured and observed data or, in other words, the precision of the model itself.

Then, in a real case, **n** may variate from a minimum value of **2** to a maximum value according to the ratio between precision level required and practical and/or economical esigences. Stability of a model generated on **n** points may be tested using a rising number **n-m** (being **m** comprised between **1** and **n-1**) of points as independent measured values for model testing.

It should be noted that **2** is the minimum sampling point number if isotopic composition is calculated respect to variables independently measured, for example temperature and amount of precipitation, through the use of methods as simple or multiple linear or non linear regression. If a gradient method is involved in calculation, minimum number of sampling points rise up to **3**: two points for gradient calculation and an intermediate point to test predicted values.

In general, a modeling procedure can be applied each time it can provide significant data for specific purpose. This means that, if in a certain area the yearly average values of $\delta^{18}O$ range from -2 δ to -10 δ, even if the standard error of estimate of the modeling procedure is 4 δ, it is possible to use the model to differentiate between two areas.

In conclusion, depending on the number of isotopic composition sampling points available, two different logical approachs are possible:

a) If only two sampling points are available, Oxigen isotopic composition variations can be related to variations of the selected independent (altitude, temperature, amount of precipitation, distance from the sea, etc.), with methods other then gradient; the model will be generated on one point and the other one will be used for testing.

b) If there are three or more sampling points, it is then possible to proceed with two different interpolation criteria. In the previous case the isotopic composition of Oxygen is associated with the selected variables by the use of statistically derived formulas or gradient methods; in the latter, interpolation is performed directly between the measured $\delta^{18}O$ values of each station, and the variation of precipitation is used only as a weighting function to calculate average values on a monthly or yearly basis. The choice between the first and the second possibility depends upon the dispersion of data that characterizes the statistical relationship between isotopic composition and selected parameters. If the differences between expected and measured values are reasonably low, it is better to use the first method; if the statistical models do not describe the system with sufficient precision, the second interpolation method works better.

Obviously, sampling points must be located considering expected spatial variation of isotopic composition. About the time frequency of sampling, the described method has been thought to work on yearly values of isotopic composition, computed from monthly sampled data. This is due either to the high dispersion of the relationships between isotopic composition and meteorological and/or geographical data.

Analyzing the case of the Madonie Mounts area (Fig. 1), on which the model has been tested, it must be noted that isotopic composition data available consist of monthly values for the year 1978 from two sampling points (HAUSER *et alii*, 1980): Scillato station (4), located at about 450 m a.s.l. on the western flank of the karst massif and P. Battaglia (5), in the central part of the area at 1650 m a.s.l..

Areal extension of the studied zone, about 30 × 30 km, and its geographical location, near the northern coast of Sicily, suggest that continentality effect can be neglected. As better explained later, the amount of precipitation and temperature show direct relationships with $\delta^{18}O$, they have therefore been selected as independent variables in the modeling procedures.

TEMPERATURE MODELING

In 1978 three temperature stations of the Italian Genio Civile operated in the areas: Cefalù (1) (30 m a.s.l.), Scillato (4) (450 m a.s.l.) and Petralia Sottana (8) (930 m a.s.l.). For each of them the monthly average temperature was calculated from the duration of day and night, using minumum an maximum monthly average temperatures (SERVIZIO IDROGRAFICO DEL GENIO CIVILE, 1978), by the formula (modified from GANDOLFI & SONCINI SESSA, 1978):

$$Tmed = (D/24) * Tmax + ((24 - D)/24) * Tmin,$$

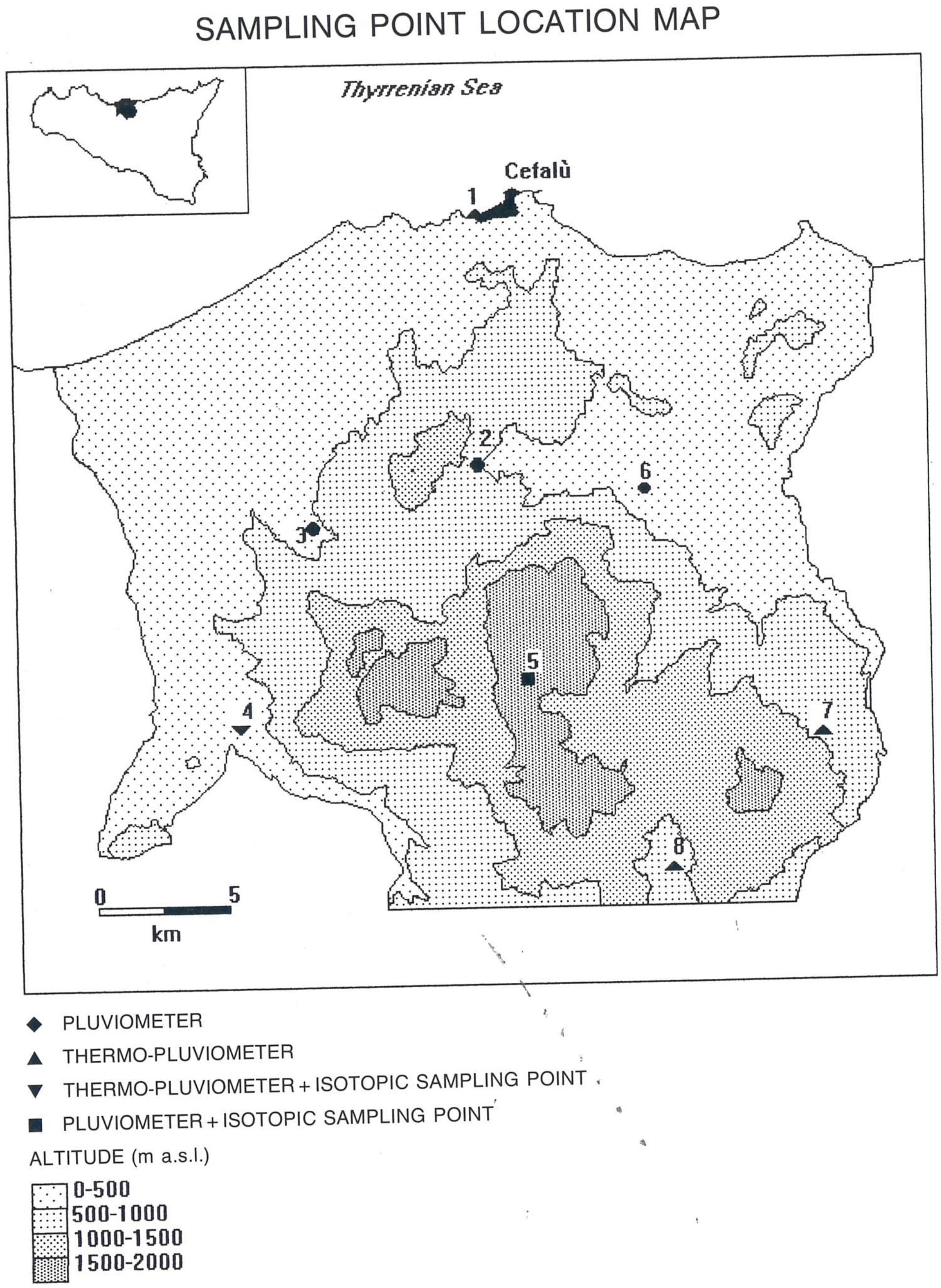


Fig. 1 — Sampling points location map.

where Tmed = average monthly temperature, Tmax = average monthly maximum temperature, Tmin = average monthly minimum temperature and D = duration of day in hours; D is derived from:

$$D = 12 + F \sin (279° + 360 * (d/366)),$$

where d is the progressive number of the central day of the mouth and

$$F = 0.1414 * L - 2.413,$$

where L is the latitude of the station; sign of L is + for northern latitudes.

Good linear relationships existing between values recorded in each station vs each other (correlation coefficients better than 0.99 with a standard error of estimation of about 0.5°C) have permitted the adoption of a vertical gradient method to extrapolate information from punctual stations to the whole area.

In order to realize a representation of surface temperature it was necessary to acquire the elevation data digitizing altitude isolines and then to convert them into isotherms by the formula (Di Natale & Madonia, 1996):

$$T = To + (A * G)$$

where To = temperature at the sea level, A = altitude and G = vertical thermic gradient.

According to the scheme showed in Fig. 2, starting from an altitude contour line map, temperature values have been derived.

The resulting coverages, one per moth, were transformed first into Tins and then into Lattices; transformation into Lattices is necessary because only using regular grids with the same spacing it is possible to perform mathematical operations between the grids.

The average yearly isotherms map showed in Fig. 3-a is an example of grid operations: it was obtained by calculation of the mathematic mean of the 12 average monthly temperature grids; the resulting Lattice was filtered with a low-pass filter to remove all the high frequency components of no physical significance. The good correspondance between isotherms and altitude contour confirms the result of temperature modeling. All calculations involved in this and in all other procedures have been executed by automatic programs written in AML (ARC/INFO Macro Language), in order to minimize execution time.

Precipitation modeling

Precipitation modeling, such as temperature, is not so easy to perform. Various methods have been developed, either deterministic (isohyetal method)

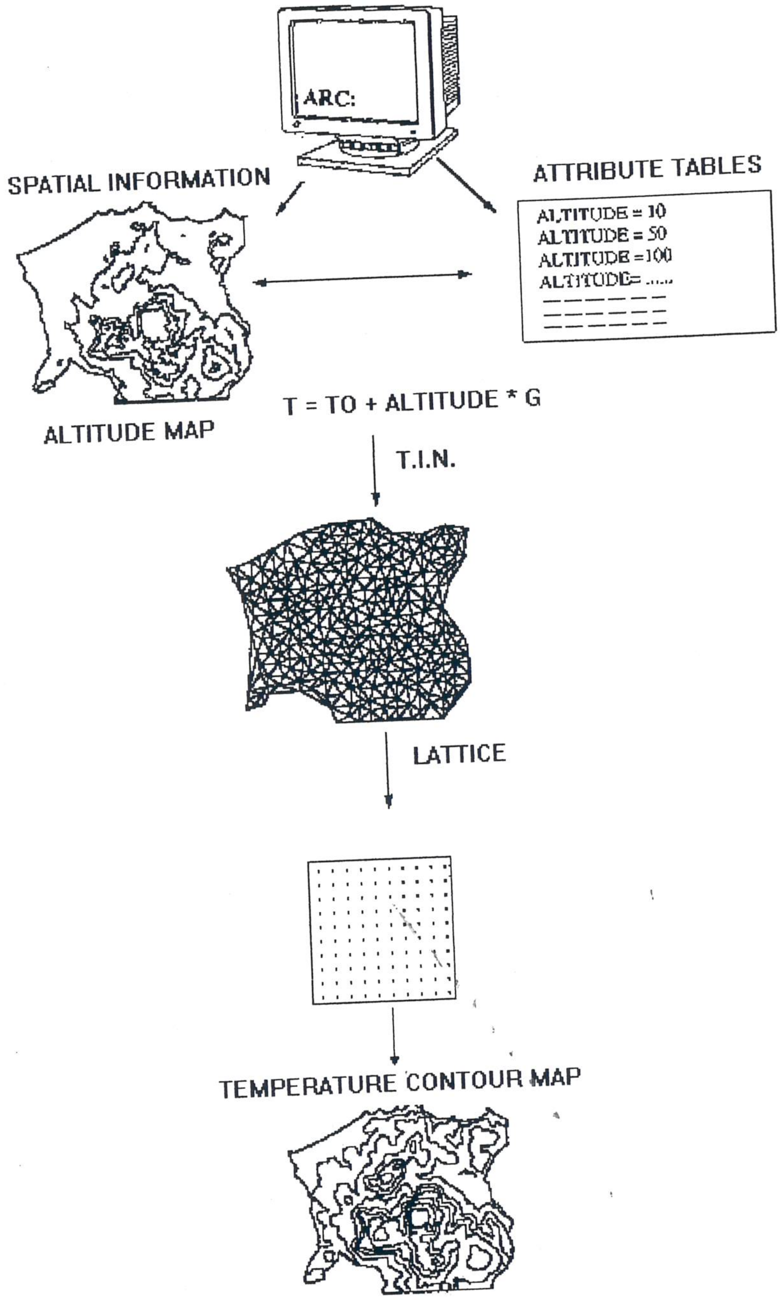


Fig. 2 — Steps of temperature calculation.

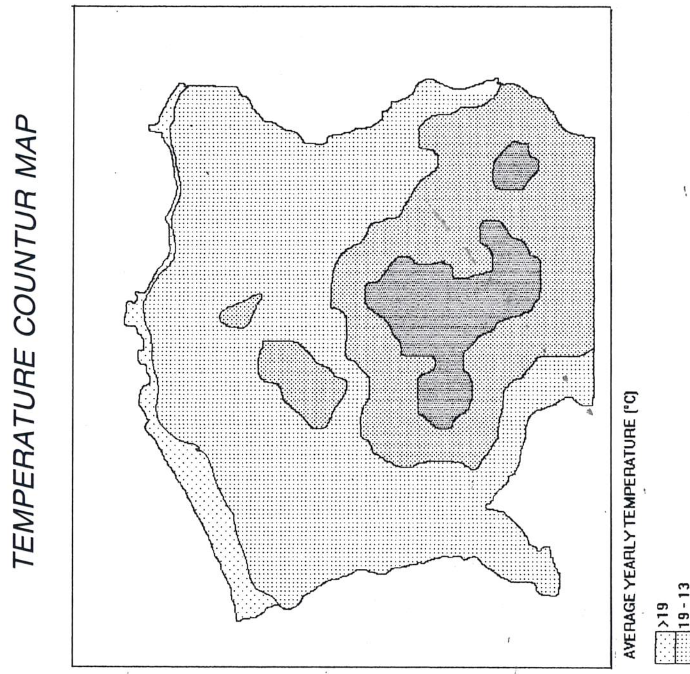


Fig. 3a — Temperature contour map.

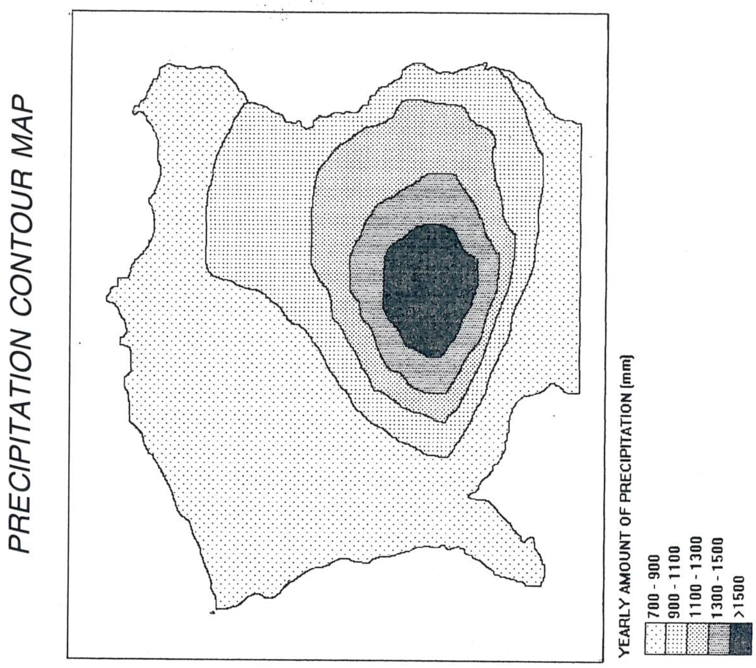


Fig. 3b — Precipitation contour map.

or stocastic (kriging method), but none of these works well; the isohyetal method has been preferred because of its simplicity, more complex methods beeing unable to enhance the quality of interpolated data.

In this case a map of 8 pluviometric stations was digitized and precipitation values for each month (SERVIZIO IDROGRAFICO DEL GENIO CIVILE, 1978) were associated in the attribute table.

The procedure to obtain the precipitation contour map is the same as for the temperature; the only difference being that the original coverage is a point coverage.

The yearly amount of precipitation map, showed in Fig. 3-b, has been obtained by the simple addition of the 12 monthly Lattices; isohyetal lines seems to be smoothly related to altitude variations, as it is expectable when precipitation events are orographically driven.

ISOTOPIC COMPOSITION MODELING

Oxygen isotopic composition data available plotted vs temperature and amount of precipitation are showed in Fig. 4; in general, low values of $\delta^{18}O$ correspond to high values of temperature and amount of precipitation and vice-versa, according to the general relationships previously discussed. Using a multiple regression method a linear equation of the type:

$$d = a * P + b * T + c$$

(where d = monthly average $\delta^{18}O$ value of precipitation, P = monthly amount of precipitation and T = monthly average temperature) was calculated. In Tab. III results of calculation for both the sampling points are showed.

Tab. III

Results of multiple regression calculations

Parameter	Scillato Station	P. Battaglia Station
a	0.001659	-0.005668
b	0.547806	0.104088
c	-14.5	-7.9
r	0.7818	0.6534
σ ($\pm\delta$)	2.13	1.3

Due to the large difference between a, b and c values computed for each station, an interpolation criterion was needed for the extension of calculations to the whole area.

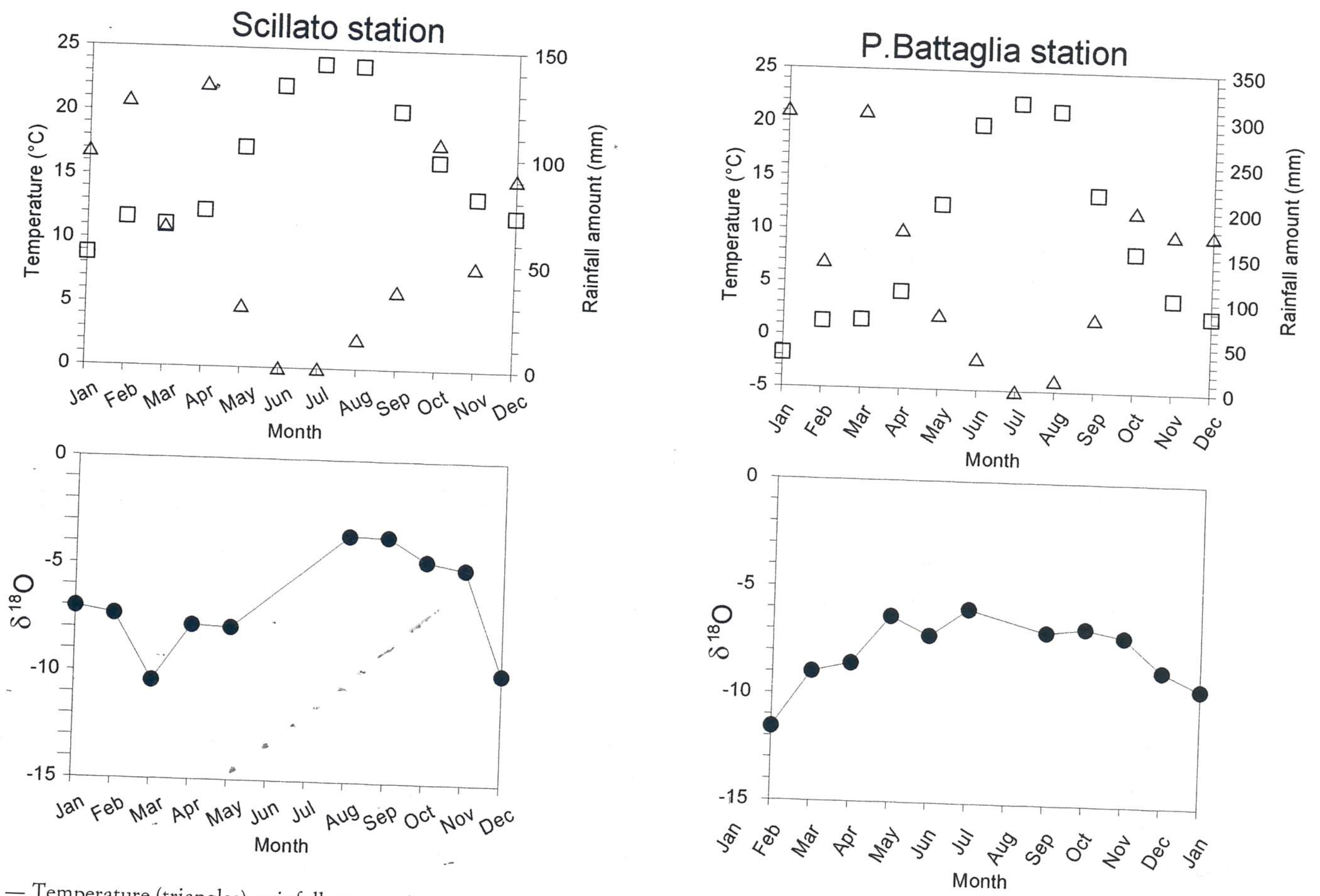


Fig. 4 — Temperature (triangles), rainfall amount (squares) and isotopic composition of precipitation (filled circles) of Scillato and. P. Battaglia stations (montly values for the year 1978).

The correlation coefficient matrix of the monthly amount of precipitation of each station vs each other (Tab. IV) clearly shows the existing relationship between the stations; all of them present a good linear relationships, with the exception of Piano Battaglia and Petralia, in which the local orographic conditions determine different mechanisms driving precipitation events. Moreover, the pluviometer installed in Piano Battaglia managed to collect correctly only liquid precipitation: real values of $\delta^{18}O$ during the cold season could be lower than measured ones, due to isotopic fractionation processes affecting the snow caps developed on the funnel during snowfalls.

Tab. IV
Correlation coefficients matrix of the pluviometric stations

Station		Cef	Isn	Col	Sci	PBa	Cas	Ger	Pet
Cefalù (1)	1	.876	.848	.881	.587	.936	.877	.718	.718
Isnello (2)		1	.866	.942	.765	.946	.931	.847	.847
Collesano (3)			1	.817	.560	.820	.786	.807	.807
Scillato (4)				1	.732	.928	.927	.799	.799
P. Battaglia (5)					1	.651	.676	.732	.732
Castelbuono (6)						1	.911	.719	.719
Geraci (7)							1	.846	.846
Petralia (8)								1	1

In the modeling of Oxygen isotopic composition a two-compartment model was then adopted; the equation computed from the Scillato data was used for $\delta^{18}O$ calculation in the whole area, except for the endoreic area surrounding the Piano Battaglia station in which the other equation was used.

From the monthly precipitation Lattices and the monthly temperature Lattices, using the multiple linear regression equation, monthly average $\delta^{18}O$ Lattices were derived.

The average yearly isotopic composition contour map, obtained by weighting the montly values with the monthly amounts of precipitation, is showed in Fig. 5.

Future improvements

As noted in introduction, the goal of this work was more the development of a logical approach to computer modeling of the isotopic composition of precipitation rather than the attempt to produce high significance data; the available isotopic composition data series were too short, both in space

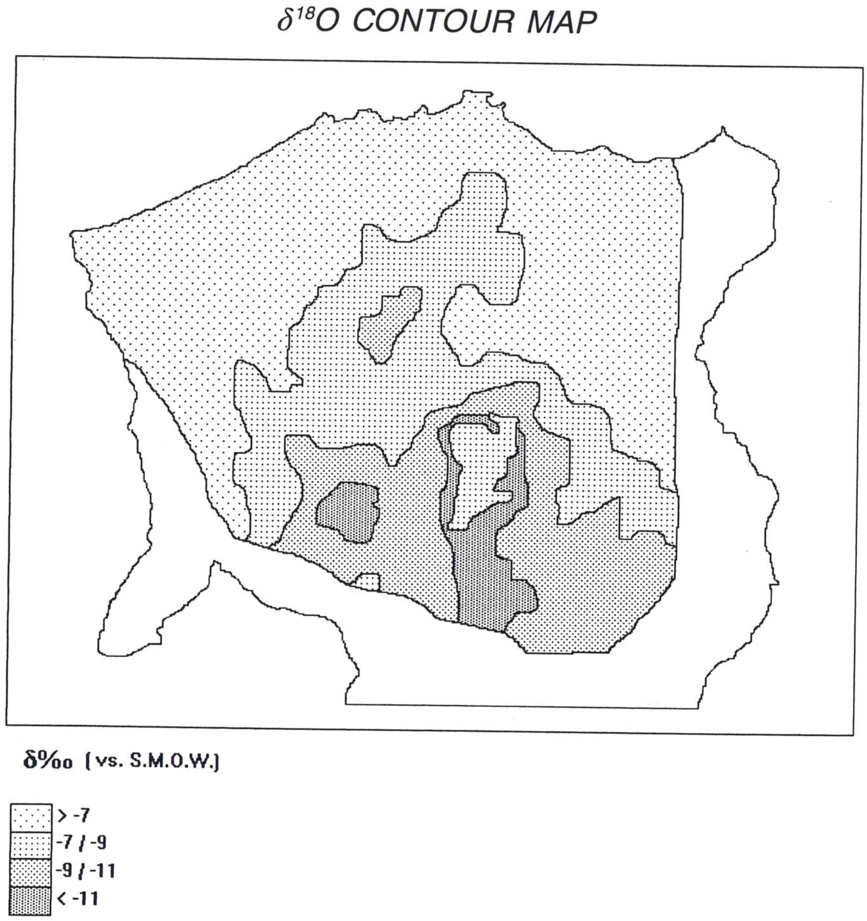
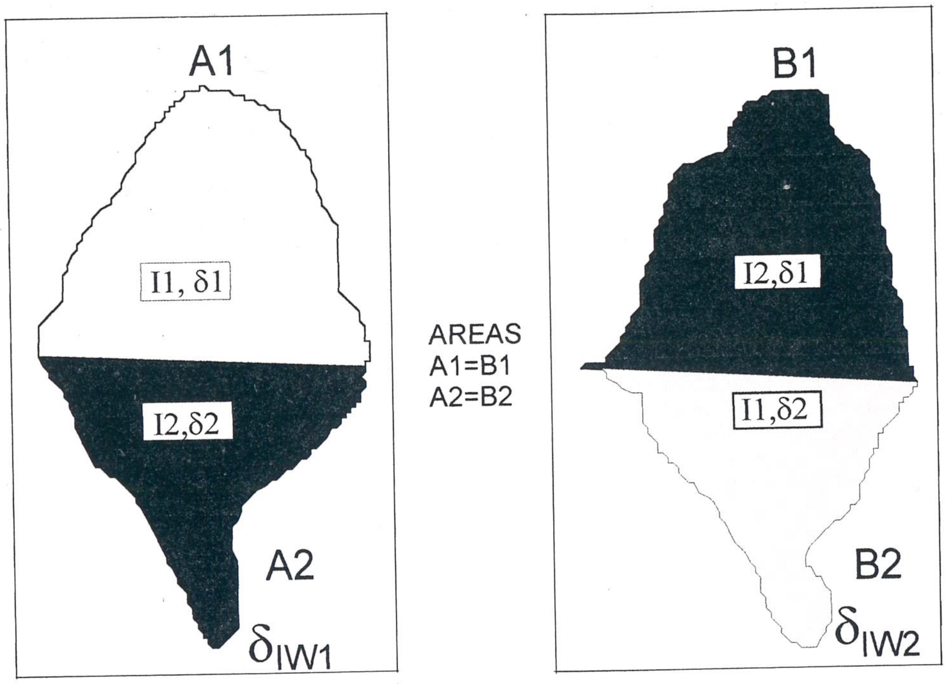


Fig. 5 — $\delta^{18}O$ contour map.



I1=0.9 / I2=0.1
δ1= –8 / δ2= –6
δIW1= -7.8

I1=0.9 / I2=0.1
δ1= –8 / δ2= –6
δIW2= -6.2

I = Average infiltration coefficients
δ = Average isotopic composition of precipitations
δIW = Average isotopic composition of infiltrated waters

Fig. 6 — Average isotopic composition of infiltrated waters in two watersheds characterized by different infiltration coefficients.

and in time, to allow for the generation of a precise and accurate model.

An other important point in the model optimization is the possibility of evaluating the average isotopic composition of infiltrated waters; in other words, if there are two watersheds characterized by the same area and the same orographic assestment, but outcropping lithology is different, even if the average isotopic composition is the same the resulting composition of infiltrated waters will be different (Fig. 6). All parameters of the hydrological balance can be easy modeled using GIS technology, allowing the development of an accurate weighing function for the calculation of isotopic composition of infiltrated waters.

BIBLIOGRAFIA

DI NATALE R. & MADONIA P., 1996 — Metodologie informatiche applicate allo studio di un'area carsica: il caso del massiccio carbonatico delle Madonie Sicilia. In: Proceedings of International Symposium on Alpine Caves and their environmental system, Asiago (Vicenza, Italia), June 1992. — Tip. Lanaro, Malo (VI).

ESRI, 1991 — ARC/INFO Users Manuals.

GANDOLFI C. & SONCINI SESSA R., 1981 — IDRO-1 Manuale d'uso. — *CLUP*, Milano.

GONFIANTINI R., 1978 — Standards for stable isotope measurements in natural compounds. — *Nature*, Lonhdon, 271: 534-536.

HAUSER S., DONGARRA G., FAVARA R. & LONGINELLI A., 1980 — Composizione isotopica delle piogge in Sicilia. Riferimenti di base per studi idrogeologici e relazioni con altre aree mediterranee. — *Rendiconti SIMP*, Varese, 36 (2): 671-680.

SERVIZIO IDROGRAFICO DEL GENIO CIVILE, 1978 — Annali Idrologici: Parte I. Palermo

YURTSEVER Y. & GAT J.R., 1981 — Atmospheric waters. In J.R. Gat & R. Gonfiantini (eds.), Stables Isotope hydrology. — *I.A.E.A.*, Vienna: pp. 103-142.

Indirizzo degli Autori — PAOLO MADONIA, Istituto di Mineralogia, Petrografia e Geochimica, via Archirafi, 36 - 90100 Palermo (I); ROCCO FAVARA & MARIANO VALENZA, IG.F./C.N.R., via Torino, 27/d - 90100 Palermo (I).