

## Mathematical simulation of karst development

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**Abstract** During the last ten years, the author has attempted to develop an algorithm for the mathematical simulation of karst and, in particular, of the spatial distribution and time evolution of karst conduits (caves). At the present stage, the general model has been formulated to forecast, with an acceptable degree of accuracy, the bidimensional distribution of the underground network, the physical relationships between the different sets of conduits, and the evolution of conduit patterns, i.e. of the underground hydrological network of karst systems. Several real systems have been simulated and case studies are presented after a general discussion of the physical principles and mathematical formulation of the problem. Boundary conditions and triggering mechanisms are discussed and special attention is given to the formulation of an adequate set of driving equations describing thermodynamic coupling and energy, mass and momentum transfer among the constitutive spaces of the karstic environment (solid matrix, pores, joints, caves) rigorously placed in hierarchical order after measurement of the characteristic lengths.

### **Simulación matemática del desarrollo del carso**

**Resumen** Durante los últimos diez años el autor ha intentado desarrollar un algoritmo para la simulación matemática del carso y, en particular, de la distribución espacial y evolución temporal de los conductos cárnicos (cavernas). En la actualidad, el modelo general ha sido formulado para pronosticar, con un grado aceptable de precisión, la distribución bidimensional de las redes de conductos subterráneos, la relación física entre los diferentes conjuntos de conductos y la evolución de los patrones de galerías; es decir, la evolución de la red hidrológica subterránea de los sistemas cárnicos. Varios sistemas reales han sido simulados y se presentan algunos estudios de casos luego de una discusión de los principios físicos y la formulación matemática del problema. Las condiciones de contorno y los mecanismos de "triggering" se discuten brindando una especial atención a la formulación adecuada del conjunto de las ecuaciones que describen el coupling termodinámico y el transporte de masa, momento y energía entre los espacios constitutivos del universo cárnico (matriz sólida-poros-grietas-cavernas) rigurosamente jerarquizados a partir de una medida representativa de la longitud característica.

## INTRODUCTION

The mathematical simulation of natural processes is a very difficult task because of: (a) the huge number of variables involved; (b) the stochastic nature of many of these variables and of the processes in which they occur; (c) the presence of nonlinear processes; (d) the absence of equations describing the mechanisms and processes that

take place within the system, the area generated by it or which act upon its boundaries, and (e) the absence or, at least, an incomplete formulation of a conceptual model capable of being developed physically and mathematically.

As well as being the most impressive feature of limestone terrain, caves are simply the main underground drainage networks of karstic regions. Although their contribution to the overall water balance of the aquifer could not be so important as that of the joints and pores, due to the differences in storage and transmissivity, cave systems move more instantaneous mass than joints and pores. They exhibit higher values of transmissivity of the whole aquifer system, lower values of storage coefficient and, of particular importance, when integrated and hydrologically active, caves represent the real flow path of groundwater, also governing the direction of underground flow in minor spaces. Whether hydrologically active or not, cave systems represent the most complex result of the interactions between geological, geomorphological, physical, chemical, climatic, hydrodynamic and thermodynamic processes at different space and time scales.

Since the early 1960s, under different approaches, several attempts to simulate the development of cave systems have been published (Eraso, 1975, 1982; Ewers, 1976; Curl, 1971; White, 1976). While numerous problems remain unsolved and other new problems have arisen from mathematical formulation or when testing under different initial and boundary conditions, the proposed models usually give unsuccessful results or show important deviations from the real system. Nevertheless, the most important result achieved is that karst and, particularly its underground drainage patterns (i.e. caves) can be mathematically modelled.

During the last ten years the author has attempted to develop an algorithm for the mathematical simulation of the spatial distribution and time evolution of karst conduits (Molerio 1982a,b,c, 1984a,b, 1985a,b,c, 1986a,b, 1988, 1989, 1990; Molerio & March, 1985; March & Molerio, 1987). At the present stage, the general model has been formulated to forecast the bidimensional distribution of the underground network, the physical relations among different sets of conduits, and the evolution of conduit patterns, i.e. the evolution of the hydrological network. Several real systems have been simulated with an acceptable degree of accuracy. Model validation is based on: (a) the continuous improvement of its physical, mathematical and conceptual basis; and (b) the hydrogeological research and speleological exploration and surveying of the simulated system.

Tested under different initial and boundary conditions, modelling has allowed: (a) the derivation or extension of different sets of the governing equations describing the development of karst conduits—in time and space; (b) forecasting of the position and some geometrical characteristics of known passages and unknown conduits; (c) forecasting of the position of springs and the extension of their underground catchment areas; (d) computation of the turnover time of groundwater and estimation of the mass balance of particular tracers or pollutants; (e) adjustment of the flow paths, head distribution and recharge estimates; and (f) testing, in particular cases, the theories developed to explain the origin and evolution of the simulated network.

The conceptual model is stochastic by nature and by definition (Molerio 1982a,b,c, 1984a,b, 1985a,b,c, 1986a,b, 1988, 1989, 1990; Molerio & March,

1985; March & Molerio, 1987). After its performance, special efforts have been devoted to derive the driving equations describing the physical governing laws (Molerio 1982b, 1986; Molerio & March, 1985), transport phenomena (Molerio 1982b, 1985a), the statistical continuity of the physical properties among the constitutive spaces (caves, joints and pores) (Molerio 1982a,b; Molerio & March, 1985; March & Molerio, 1987) taking into account their inertia (memory) (Molerio 1985b), time-dependence (Molerio, 1984b), the influence of the scale factor (Molerio, 1984a), entropy variation (Molerio 1988, 1989, 1990), linear and nonlinear feedback loops (Molerio 1985b), and the interaction between the involved forces and fluxes (Molerio 1988). Mass, moment and energy transfer were initially solved in terms of transport functions and, in some cases, as phenomenological coefficients derived by nonequilibrium thermodynamics (NET). Within the system, work has been described by energy-dissipation functions (EDF) among the constitutive spaces as far as they could be defined like self-regulated energy-dissipation functions and mass, moment and energy transfer functions are described by multiple thermodynamic coupling.

Triggering dissolution effects are considered by relating thermodynamic coupling among chemical reactions and vectoral phenomena in anisotropic media. Thermodynamic fluctuations, which in turn could be derived from the time and spatial coincidence among the onset of the phenomenological coefficients, the nonlinear high velocity fluxes and related forces, and the increase of the dissolution rate, was computed as single fluctuations in random time. Therefore, boundary conditions should provide that initial time is very much shorter than total time and, when a approaching infinite probabilities of the functional extremes should be considered negligible.

Although the model needs sustained improvement, the results obtained are promising. Conceptually, our model has been developed involving several principles from the theory of automatic control of nonlinear feedback self-regulated systems stressed by random inputs. Nonequilibrium thermodynamics is the governing physical basis so the model is largely based on statistical physics.

## CONCEPTUAL MODEL AND THEORETICAL PROBLEMS

The conceptual model defines karst as a dynamic system. Thus it is a physical entity subjected to the action of five main laws (Molerio 1985b):

- conservation of energy;
- conservation of a spatially coherent identity;
- least work;
- equal work distribution;
- increase of entropy.

As has been previously pointed out (Molerio, 1985b, 1989), the conceptual model describes karst systems by the following properties:

- (a) thermodynamically, karst is an open system interacting with the surrounding media;

- (b) variables describing the system's physical properties show a progressive tridimensional anisotropy;
- (c) for any basic measure of a characteristic length (area, volume, length, effective diameter) the karstic space is rigorously organized in hierarchical order, and four types of constitutive spaces developed there, generically designed—in decreasing order of characteristic length—as caves, joints, pores and solid matrix;
- (d) each of the constitutive spaces exhibits their own flow domain and, among them, an active exchange of mass, moment and energy takes place;
- (e) according to this the physical properties field is structured and defined for each space;
- (f) responses to both external or internal (natural or artificial) inputs of mass, energy and moment are hierarchically modulated by the system's internal structure and capability to assimilate stresses;
- (g) the scale factor exerts a strong influence on the physical meaning and stochastic behaviour of the physical properties;
- (h) within the system, work development produces self-regulated energy dissipation structures feeding back the whole set of processes;
- (i) thus, the system and in particular, the physical properties defining it are highly time-dependent at different space and time scales;
- (j) the karstification process is irreversible, its evolution is unidirectional towards increasing levels of entropy.

Until now, several theoretical problems remain undefined and, of course, unsolved mathematically, but the conceptual model itself is suitable for physico-mathematical analysis and in particular for stochastic modelling. As a logical derivation of our conceptual model, a working hypothesis for conduit simulation was developed (Eraso, 1982; Ewers, 1976; Curl, 1971; Molerio, 1982a,b, 1986a,b, 1989, 1990; Egemeier, 1969; Carnahan, 1976). The main facts are the following:

- (a) Karst conduits are linear, planar or areal spaces, oriented along privileged linear planes, mainly joints, stratification planes and pores. Planar and areal structures are less important in number although they can orientate karst conduits. Joint-governed karst conduits are even more statistically significant than any other kind of surface.
- (b) Linear topologies are often developed along the intersection of surfaces.
- (c) In terms of conduit (i.e. cave or joint enhancement) development, these surfaces are of two kinds and occur in defined spaces: a zone of maximum solvent concentration (MSC) and a zone of maximum flow concentration (MFC).
- (d) Generally, MSC surfaces are horizontal or sub-horizontal and defined by the geochemical evolution of the system, the supply sources and the residence time of water within the system.
- (e) MFC surfaces are usually sloping surfaces, sometimes with a very steep gradient, but uncommonly horizontal.
- (f) At the intersection between MSC and MFC surfaces, major fluid volume and major solvent concentrations occur, so there is a greater probability of solution and, of course, of cave development.

- (g) Work done at the intersection points does not reach thermic equilibrium. The exchange of mass, moment and energy leads to the progressive development of an open system in which entropy increases from an initial time where the system ceased to be a closed one.
- (h) The MFC surfaces are found in the direction of the velocity component of hydraulic conductivity; lateral flow occurs in the direction of the hydraulic gradient component. Therefore, the maximum probability of cave development could be determined knowing the distribution of each component. This means that the development of an underground net of conduits in karst systems can be forecast in terms of the random variables characterizing the mass, moment and energy transfer allowing the use of spectral and covariance methods to account for their space variability. This is in addition to those required to define the probability distribution of the variables involved, and also to describe the noisy boundary conditions, distributed in time and space, since they are additional sources of stochasticity for the system's response.
- (i) Karst conduits are excavated in selected intersection points for a given probability, not in all of them. This apparent contradiction is solved in terms of another set of a probabilistic nature. The direction of excavation and then the probabilistic distribution of those selected paths are governed by the second law of thermodynamics so excavation will take place *only* in the direction of maximum entropy increase.
- (j) The introduction of the probabilistic nature of entropy in the model allows one to define that each of the system's constitutive spaces are developed according to the principles of nonequilibrium thermodynamics. From karst conduits (caves) to solid matrix, decreasing values of the energy dissipation function should be found and the set of phenomenological equations has to be solved for each of the involved spaces.

In our model the constitutive spaces are treated as continua (Molerio, 1982a, 1985a; Molerio & March, 1985; March & Molerio, 1987). Validation of this hypothesis depends on the demonstration of the statistical continuity of the physical properties scaled after characteristic length (Molerio, 1985a; Molerio & March, 1985). Such scaling and statistical continuity should be defined in the real world. Thus, the Elementary Representative Area (AER), volume (REV) or length (REL) (Molerio, 1985b) have to account for the distortion derived of the scale factor (Molerio 1984a,b), not only in terms of the absolute value of a given property, but in its direction; for the spatial variance or covariance due to the different degree of heterogeneity considered (Molerio, 1982a,b, 1985a,c, 1986a) and also, for the time-dependence of the given physical property (Molerio, 1984) and of the field involved (Molerio 1984, 1986b).

Mass, energy and momentum transport processes among equivalent continua are solved, for each of the involved spaces, performing a set of equations describing the transport functions (Molerio, 1985b; Molerio & March, 1985; March & Molerio, 1987). At the same time, work producing self-regulated energy-dissipation structures (EDS) is assessed after the derivation of a set of equations describing, for the involved spaces within the system, the energy-dissipation function.

The interaction between forces and fluxes can not be mathematically treated if NET principles are not generalized to the macro scale. The main problem is that the physical basis of the NET, the Onsager's Reciprocal Relations (ORR) are not rigorously described for the macro movement. Nevertheless as a first approach, it was considered that each randomly distributed space is characterized by a value or a range of values for the energy-dissipation function (EDF). Those values should be initially controlled by the volumetric rate of entropy production. In addition, the EDF has to be statistically continuous in time and space because each new EDS has to comprise more entropy than the previous (Molerio & March, 1985; March & Molerio, 1987; Molerio, 1988; Carnahan, 1976).

It is then a valid approach combining the equations of mass, moment and energy balances with the Gibbs equation in order to characterize the system by obtaining an adequate formulation for the entropy balance. In fact, the symmetric property of the tensorial field describing the phenomenological coefficients is supposed. Such an approach allows one to obtain a general equation for the system's entropy change as a function of the potential difference and the chemical affinity of the main reactions. Forces and fluxes considered are: (a) heat transport; (b) volumetric flux; (c) dispersive-diffusive flux; (d) electric conductivity; and (e) chemical affinity. They were linked with transfer and EDFs by multiple thermodynamic coupling.

The first results showed important deviations due to several sources of stochastic uncertainty. The most important result was of a thermodynamic nature and is related with the time-varying initial and boundary conditions. In particular it concerns those conditions producing the transformation of an initial closed or isolated, reversible system, without external stresses or perturbations into an open irreversible system, satisfying the properties mentioned above. A special effort was made to characterize the random inputs, both external or produced by the system, (a) in terms of its filter capability to those inputs; (b) to define the extent of those effects in case they were able to produce thermodynamic fluctuations; (c) to differentiate the stationarity of the random signals; and (d) to solve the system's response in the direction of the increasing entropy (Brown, 1970; Terlietsky, 1975; Carnahan, 1976; Molerio, 1990a,b).

One of the effects involved in the change of such thermodynamic systems is kinetic triggering (Howard, 1964; Howard & Howard, 1967; Thrailkill, 1968; Brown, 1970; Curl, 1965; Morse & Berner, 1972; Berner & Morse, 1974; Terlietsky, 1975; White, 1976). It seems that this group of effects is partly responsible for a thermodynamic fluctuation and, in any case, the problem is first solved theoretically (Howard, 1964; Howard & Howard, 1967; Thrailkill, 1968; Brown, 1970; Curl, 1965; Morse & Berner, 1972; Berner & Morse, 1974; Terlietsky, 1975; White, 1976; Netushil, 1987). It should be kept in mind that any macroscopic state is a function of the microscopic state due to the irreversibility of the micromovement equations. Thus, any system could move spontaneously from one microscopic state to another and *vice versa* without external coactions. The same could be said for the macroscopic state, but micromovement irreversibility defines that without external coactions spontaneous movement is only unidirectional. Commonly, this paradox is solved considering that macroscopic irreversible

movement equations are valid only since an initial time before which the system was isolated. On the contrary, in permanent isolated systems, irreversible processes can only take place as the result of a spontaneous fluctuation (Terlietsky, 1975).

The most important point is that entropy increase can only take place after that initial time. For an isolated system, macroscopic equations describe reversibility for an infinite time interval because entropy first decreases and later increases. For a non-permanent isolated system the initial time is physically relevant; after that time, macroscopic equations can only conduct towards entropy increase without any contradiction with the microscopic irreversibility (Terlietsky, 1975).

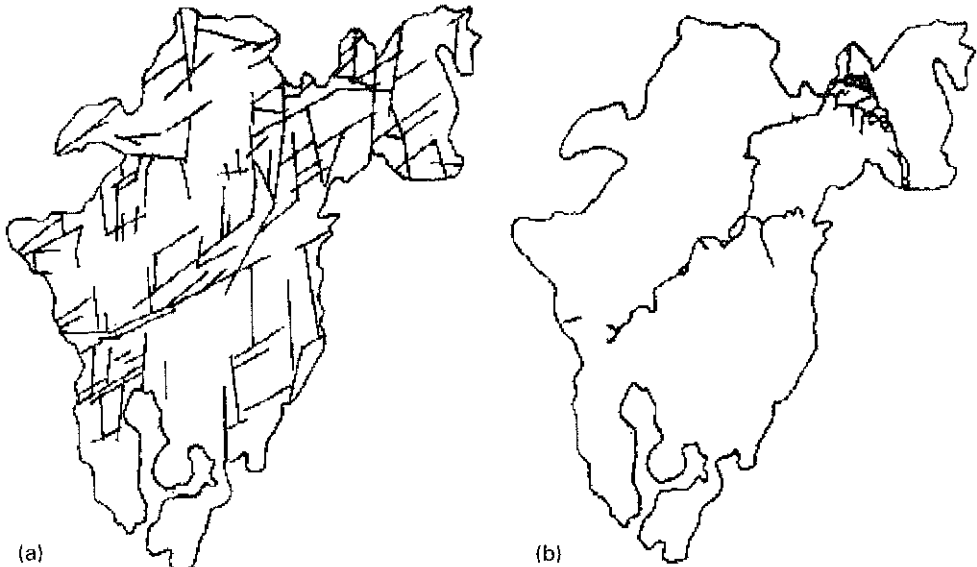
The remaining problem concerns the definition of the set of mechanisms producing perturbations in the quasi-stationary equilibrium state of the system. It seems logical to suppose that the privileged development of some conduits with respect to others should be due to a combination of the dissolution kinetics, the flow regime and the increase in entropy. In fact, results obtained by several authors (Howard, 1964; Howard & Howard, 1967; Thrailkill, 1968; Ewers, 1976; Curl, 1965, 1971) seem not to be in perfect agreement. This was recently discussed in some detail (Molerio, 1995) leading to the conclusion that some kind of triggering mechanism could explain, at least in part, the change in thermodynamic state.

In our approach, dispersivity is defined as a fourth-rank tensor while the dispersion coefficient is a second-rank tensor. Transforming the dispersion coefficient into a phenomenological coefficient in terms of solute velocity causes the flow velocity to vanish in a closed system, but the rate of solute dispersion remains influenced by the porous matrix or the conduit in the field of zero flux. A combination of transport and phenomenological terms allows one to relate solute properties accounting for the dependence of chemical potential with respect to concentration. Therefore, the thermodynamic fluctuations, due to the coincidence of the onset of the dispersion phenomenological coefficients, the nonlinear high-velocity flow and the increase of the dissolution rate, are computed as single pulsations of certain time span at a random instant. This can be done provided that initial time is very much shorter than total time, as the probability of the functional extremals is negligible when total time approaches infinity.

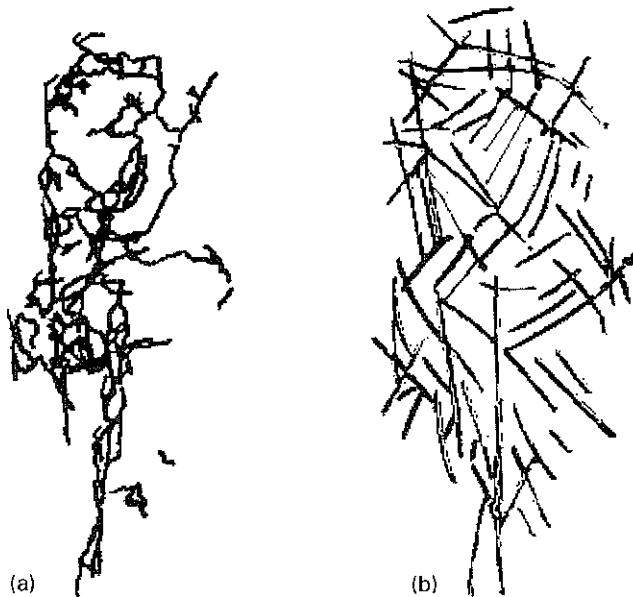
## **FINAL REMARKS**

The development and improvement of the simulation model has been validated on real systems. Figure 1 shows two examples of model application in different environments. Figure 1(a) represents the theoretical conduit development at the Sierra de San Carlos in Western Cuba, an isolated tower karst hill where explored cave passages reach 30 km, as shown in Fig. 1(b). Coincidence between surveyed passages and the simulated network reaches 94% for a confidence level of 95%. According to the model, present knowledge of the real system accounts only for 46% precision.

Figure 2(a) shows the simulation results for the Dent de Crolles Plateau in the French Alps where the known 52 km of the Dent de Crolles cave system is



**Fig. 1** (a) Simulated cave development of the Sierra de San Carlos, Pinar del Río, Cuba (Majaguas-Cantera cave system). (b) Surveyed underground passages of the Majaguas-Cantera cave system, Pinar del Río, Cuba.



**Fig. 2** (a) Surveyed and (b) simulated underground passages of the Trou du Glaz cave system, Dent de Crolles, France.

developed. Here, the very high performance of the model accounts for its reliability when compared with the surveyed underground network (Fig. 2(b)). Here, the coincidence between surveyed passages and the simulated network accounts for

**Table 1** Reliability indexes for model validation (confidence level 95%).

System	Total length of surveyed passages (km)	Total precision	Precision with respect to the surveyed passages (length+orientation)	Potential simulated length (km)	Total CV (length+orientation)	
					Real	Simulated
S. de San Carlos	30	83%	94%	65	0.52	0.64
Dent de Crolles	52	80%	92%	74	0.48	0.62

92% precision while present knowledge of the real system is very high (70%). Table 1 comprises some of the characteristic parameters of model validation. The selected indexes for the stochastic deviation of errors were spatial variance, length and orientation coefficient of variation (CV), and standard deviation of cumulative lengths in a defined orientation interval. For the sake of simplicity only the CV for both the real and the simulated system are given. Differences in CV indicate an increased heterogeneity of the system when potential conduit length is higher than actual or known length. For practical purposes, such as an assessment of regional transmissivities or groundwater monitoring networks design, the change in the class of heterogeneity should account for adjustments in the correlation length and variogram parameters when four heterogeneity classes (one for each constitutive space) are defined (Molerio, 1995). The Fisher test was applied for significance assessment of the different variances and the Kolmogorov-Smirnov test was applied for the assessment of statistical significance between real and simulated length and orientation of conduit segments. Without trends, the covariance function is the complement of the semivariogram with respect to variable variance.

Several problems need careful attention in the future. For example, the introduction of a triggering mechanism of Berner & Morse's type, as developed by White (1976), simplifies computational processes while disregarding the effects of physico-chemical retardation mechanisms. Another theoretical problem concerns the extension of Curie's Theorem, that prescribes thermodynamic coupling between chemical reactions and vectorial phenomena in anisotropic media. The boundary value problem between dispersion and diffusion, in the case of the development of residual diffusion at very low or zero velocities, still remains unsolved. A special problem is derived from the intrinsic nature of NET and is related to the impossibility of a direct measurement of phenomenological coefficients corresponding to thermodynamic coupling phenomena at macroscale levels.

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