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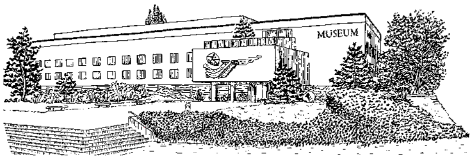

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An "Equation of state" for the morphology of Jurassic ammonites: a multidimensional law based on classical dimensions

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Abstract

Characterization of the morphology of the ammonite shell is an old, relevant and open problem in ammonitology. Since many years ago the morphology and growth of ammonoids has alternatively been described in terms of the logarithmic law. However a description in terms of the variables or dimensions most commonly accessible and used (D: diameter or size; U: umbilical width; H_1: whorl height; H_2: whorl ventral or apertural height; and W: width of whorl section) is still missing due to the lack of relationship between these variables with those of the logarithmic law. In this paper we have found the relationship between the spiral logarithmic law and a multidimensional law which we have called the equation of state of the post-embryonic shell of Jurassic ammonites. This law is written in terms of D, U, H_1 and H_2 and has been tested on 25 species of Middle and Late Jurassic ammonites of the superfamilies Perisphinctoidea, Stephanoceratoidea and Haploceratoidea. Results obtained show an agreement with only 1-22% of uncertainty between observations and predictions, thus describing, at least, the 80-90% of the morphology of the studied ammonites. It was also concluded that H_1/D and H_2/H_1 are fundamental parameters for describing the basic form and growth of ammonites in the equatorial plane.

Key words

Ammonites, Jurassic, Morphology, Multidimensional model.

Resúmen

Una ecuación de estado de la morfología de amonites jurásicos: ley multidimensional basada en las dimensiones clásicas.- La caracterización de la morfología de la concha de amonites es un viejo y relevante problema en amonitología que se mantiene abierto. Desde hace varias décadas la morfología y el crecimiento de los amonites han sido alternativamente descriptos en términos de la ley logarítmica. Por otra parte una descripción en términos de las variables o dimensiones más comúnmente accesibles y usadas (D: diámetro ó talla; U: amplitud umbilical; H_1: altura de vuelta; H_2: altura ventral de vuelta ó altura apertural; y W: ancho de la sección de vuelta) no ha sido desarrollada aún debido a la falta del conocimiento de la relación entre dichas variables con aquellas de la ley logarítmica. En este trabajo se presenta una relación entre la ley logarítmica espiral y una ley multidimensional que denominamos ecuación de estado de la concha post embrionaria de amonites jurásicos. Esta ley se presenta escrita en términos de D, U, H_1 y H_2, y ha sido ensayada sobre 25 especies de amonites del Jurásico medio y tardío de las superfamilias Perisphinctoidea, Stephanoceratoidea y Haploceratoidea. Los resultados obtenidos muestran un ajuste ó acuerdo con sólo 1-22% de error entre observaciones y predicciones, describiendo por lo tanto, al menos, el 80-90% de la morfología básica de los amonites en el plano ecuatorial.

Palabras clave

Amonites, Jurásico, Morfología, Modelo multidimensional.

INTRODUCTION

Ammonoids are fossil cephalopods whose shells preserve a large part of the history of its ontogeny and a significant part of the anatomic organization in the successive volutions or whorls, from the embryonic chamber or protoconch to the terminal adult border or peristome. It is well known that the ammonite shell may be assimilated to a coiled cone thus described as a logarithmic spiral. It is divided in three portions: (1) the protoconch, (2) the phragmocone, segmented by septa, and (3) the bodychamber alocating the soft body; the last two portions conform the conch (ARKELL, 1957). They grew adding segments, at a poorly known rate in time, changing the proportions between dimensions by differential allometric growth that is commonly described as discrete developmental and growth stages. Literature available is vast, for simplicity we refer the reader to the papers by BASSE (1952), ARKELL (1957) and BUCHER *et al.* (1996), which, moreover, contain representative lists of references.

Basic morphology of the conch of the planispiral

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ammonites may be described by some few dimensions whose relationships define a wide spectrum of different morphotypes. The study of these relationships may provide insights on developmental and evolutionary patterns and processes of morphological changes. Moreover the understanding of the morphogenetic patterns which produce the morphologic variability is crucial for distinguishing between intra- and interspecific variation what allows reliable definition of species. It requieres the quantification of these relationships between dimensions, mainly in the form of models which can be expressed by approximate mathematical laws.

There exists a strong morphological correlation among the dimensions of the ammonite shell, that has been historically evaluated by means of studies of correlation between pairs of dimensions as variables, or featuring multivariate statistical studies. Correlations are most frequently high according to the existence of some unknown multivariate law of relative growth. Perhaps the most clear and simple indication of morphologic correlation among the shell dimensions is that described by the Laws of Covariation of BUCKMAN (1892), which were studied by WESTERMANN (1966) and more recently revisited by CHECA *et al*. (1997) and HAMMER & BUCHER (2005). Quantification of the ammonite morphology by means of the parameters of the log-spiral law has been attempted by many authors based on the geometric nature of the shell (see LANDMAN, 1987 and references therein). Nevertheless this approach has not been possible using the system of dimensional variables typically adopted by ammonitologists after ARKELL (1957) (see Fig. 1, right), since the relationships between these latter and the parameters of the log-spiral law are not well known. The main gap is related to the overlapping of the whorls developed by most ammonoids from the Devonian to the Cretaceous. This important feature called involution is what diferentiates the log-spiral (non-overlapping) from the geometry of most ammonites with overlapped whorls.

We have worked to override this gap, trying to write the log-spiral law in terms of the dimensional variables commonly used, based on several species of Jurassic ammonites. The objective of this paper is to present some relevant results of this research, mainly in the form of an equation which relates most of the classical dimensions as metric variables. We have called this equation, the equation of state for the post-embryonic morphology of Jurassic ammonites.

MATERIAL AND METHOD

The material belongs to 25 species covering a wide range of the Suborder Ammonitina (Ammonoidea), representing the most typical morphologies within the superfamilies Stephanoceratoidea NEUMAYR, 1875, Haploceratoidea ZITTEL, 1884 and Perisphinctoidea STEINMANN, 1890 (Fig. 2). Dimensions used are defined in Fig. 1 (right side): D, U, H_1, H_2, and W, which define the morphospace $\mathbf{A}^{(5)} = \{D, U, H_1, H_2, W\}$. They are quantified as metric

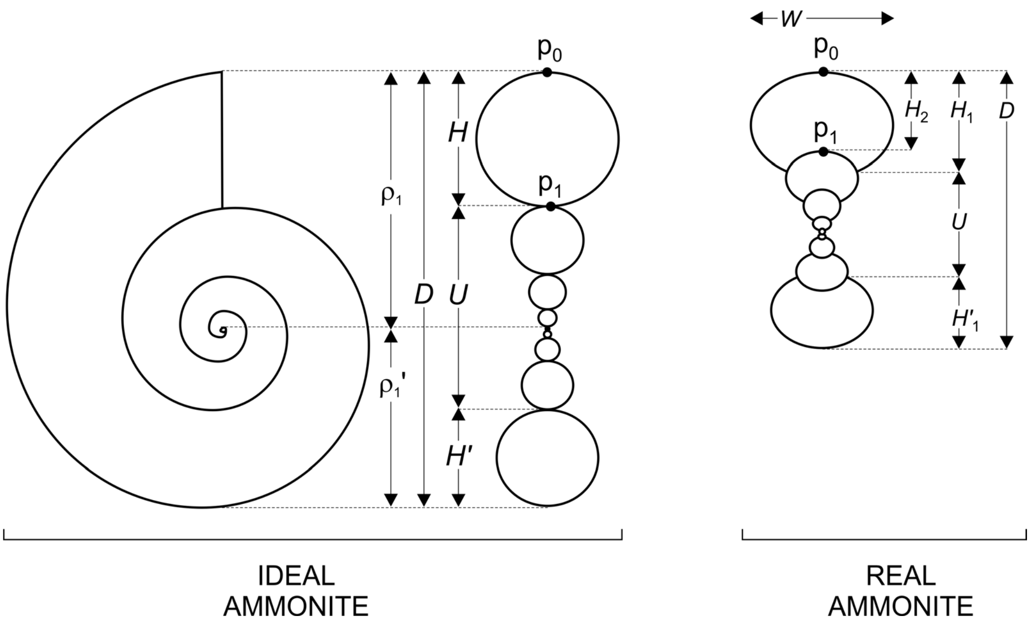

Fig. 1: Dimensions of the ammonite as used in this paper. Left: equatorial and transverse planes of an ideal or theoretical ammonite with non-overlapping whorls. Right: real ammonite with whorls overlapping each other. The number of whorls is the same in both figures.

variables consisting of distances between points. Measurements, mostly taken between ribs, are considered for $D \geq 3$ mm only, excluding in this form the ammonitella. In some cases we have obtained measurements for both sexual dimorphs ([M]: macroconch-female and [m]: micrococonch-male). Samples are heterogeneous in the sense that some of them include specimens measured for several times along their ontogeny (see Table 1). Mean values (arithmetic means) are noted by $\langle\ \rangle$.

The test, that is the original shell diagenetically replaced, may be present in ammonites but most frequently is lost partially or totally during diagenesis, during collection in the field or during preparation of the fossils in the laboratory. Test thickness is variable and changes during ontogeny like any other feature of the shell (see WESTERMANN, 1971 for details). We have not considered the presence or absence of test in outermost whorls but it was included when measuring the inner whorls.

Table 1: Relative dimensions of the ammonites studied and predictions of U/D based on the means and individual values after processing by equation (1), tests 1 and 2. Symbols and abbreviations as explained in text. N: number of specimens; n: total number of measurements. Measurements considered are all for $D \geq 3$ mm. $\varepsilon(\%)$: percentual relative error of estimation using equation (2); $\varepsilon'(\%)$: percentual relative error of estimation using equation (9) (not including corrective factor).

Species	N	n	D	$\langle H_1/D \rangle$	$\langle H_2/H_1 \rangle$	$\langle W/D \rangle$	$\langle U/D \rangle_{obs}$	$(U/D)_{pred}$	$\varepsilon(\%)$	$\langle U/D \rangle_{cloud}$	$\varepsilon'(\%)$
Stehnocephalites gerthi (SPATH, 1928) [M]	53	150	3.6 – 134.5	0.440	0.573	0.621	0.215	0.187	13.0	0.191	46.5
Stehn. crassicostatus (RICC. & WEST., 1991) [M]	5	6	43.6 – 106.9	0.421	0.624	0.491	0.264	0.214	19.2	0.221	27.1
Eurycephalites gottschei (TORQUINST, 1898) [M]	18	35	3.8 – 80.3	0.484	0.548	0.636	0.127	0.144	13.7	0.150	109.6
Eurycephalites gottschei (TORQUINST, 1898) [m]	14	26	4.4 – 34.0	0.460	0.613	0.602	0.154	0.173	12.2	0.177	88.8
Eurycephalites rotundus (TORQUINST, 1898) [M]	7	11	3.1 – 37.0	0.488	0.617	0.572	0.137	0.149	9.2	0.153	91.3
Eurycephalites extremus (TORNQUIST, 1898) [M]	4	4	8.3 – 99.9	0.466	0.571	0.668	0.159	0.163	2.1	0.168	79.5
Lilloettia steinmanni (SPATH, 1928) [M]	5	5	10.0 – 60.5	0.522	0.605	0.611	0.120	0.122	1.9	0.128	91.2
Macroceph. macrocephalus (SCHLOTHEIM, 1813) [M]	1	18	3.5 – 204.6	0.469	0.652	0.515	0.210	0.173	17.7	0.176	34.6
Macrocephalites chrysoolithicus (WAAGEN, 1875) [M]	1	18	3.7 – 246.0	0.459	0.643	0.742	0.209	0.180	14.1	0.183	40.0
Choffattia aff. *neumayri* (SIEMIRADZKI, 1898) [M]	9	9	82.0 – 31.0	0.311	0.779	0.307	0.446	0.392	12.1	0.393	6.3
Perisphinctes vicinus HAAS, 1955	36	36	4.4 – 50.7	0.348	0.742	0.485	0.402	0.330	18.0	0.333	5.8
Perisphinctes paneaticus NOETLING, 1887	41	41	4.8 – 23.9	0.394	0.842	0.527	0.346	0.308	10.8	0.309	6.4
Perisphinctes bernensis DE LORIOL, 1898	67	67	3.5 – 40.9	0.372	0.634	0.601	0.339	0.271	20.1	0.278	16.6
Euaspidoceras hypselum (OPPEL, 1863) [M]	3	4	8.8 – 113.0	0.387	0.898	0.502	0.369	0.338	8.3	0.338	2.1
Gravesia gravesiana (D'ORBIGNY, 1850) [M]	3	3	315.0 – 367.0	0.322	0.738	0.350	0.400	0.364	9.2	0.364	14.9
Euvirgalithacoceras malarguense (SPATH, 1931) [M]	5	9	33.3 – 184.0	0.354	0.763	0.322	0.397	0.329	17.1	0.330	5.3
Catutosphinctes araucanense (LEANZA, 1980) [M]	2	3	29.6 – 192.0	0.325	0.790	0.346	0.431	0.377	12.7	0.378	5.6
Lissoceratoides erato (D'ORBIGNY, 1847)	3	3	9.5 – 52.0	0.470	0.809	0.290	0.273	0.214	21.8	0.214	2.7
Scaphitodites scaphitoides (COQUAND, 1853)	37	37	5.5 – 14.1	0.480	0.676	0.434	0.169	0.168	0.7	0.178	60.2
Taramelliceras richei (DE LORIOL, 1898) [M]	61	61	5.1 – 15.7	0.541	0.711	0.336	0.149	0.127	15.1	0.128	41.1
Taramelliceras hermonis (NOETLING, 1887) [M]	65	65	4.7 – 39.6	0.543	0.709	0.393	0.153	0.125	18.2	0.128	36.8
Creniceras renggeri (OPPEL, 1863) [m]	10	10	9.9 – 21.3	0.485	0.745	0.280	0.191	0.181	5.3	0.191	39.1
Hecticoceras socini (NOETLING, 1887)	52	52	3.8 – 37.3	0.413	0.860	0.325	0.338	0.292	13.5	0.292	1.9
Hecticoceras kersteni (NOETLING, 1887)	5	5	5.9 – 40.7	0.452	0.843	0.260	0.300	0.244	18.8	0.248	0.1
Hecticoceras schumacheri (NOETLING, 1887)	34	34	3.3 – 33.7	0.396	0.839	0.320	0.362	0.304	16.0	0.306	0.7
Pseudolissoceras zitteli (BURCKHARDT, 1903) [M]	10	16	15.0 – 59.8	0.490	0.761	0.330	0.185	0.181	2.4	0.184	40.6

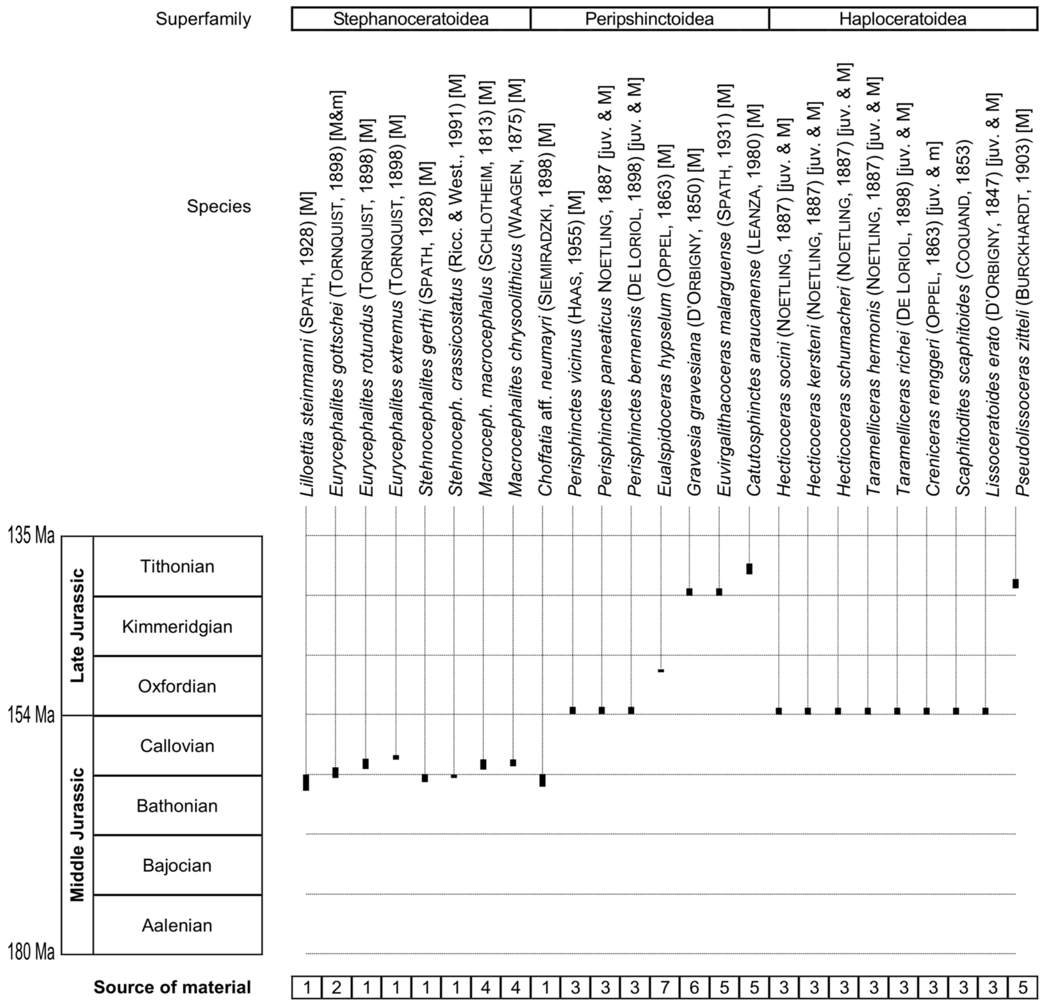

Fig. 2: Geological age of the ammonites used in this study. Geochronology in Ma (= 10^6 years) after ODIN & ODIN (1990). Origin of material: (1) PARENT (1998), (2) PARENT (1997), (3) HAAS (1955), (4) THIERRY (1978), (5) unpublished material from Picún Leufú, Cerro Lotena, Pampa Tril and La Amarga localities of the Neuquén-Mendoza Basin, Argentina (Museo Olsacher, Zapala), (6) unpublished material from Gräfenberg, Germany (col. Armin SCHERZINGER, Hattingen), (7) unpublished material from Swabia, Germany (col. Laboratorio de Paleontología y Biocronología, Universidad Nacional de Rosario, donated by Victor SCHLAMPP).

For derivation of the equation of state (a mathematical model) we have followed theoretical, phenomenological and statistical steps based on the geometric properties of the ammonite shell and empirical observations on several specimens of a moderately large number of species.

Our study is mainly based on the dimensions which are usually available in fossils, avoiding the use of spiral radius and other measurements as those defined by RAUP (1961, 1966) which can not actually be measured but in exceptional cases. Dimensional quantities are transformed into dimensionless quantities such as U/D, H_1/D, H_2/D, H_2/H_1 and W/D. These quantities are instantaneous character-state measurements (PARENT, 1997), irrespective of any growth model or pattern. Moreover, they are very useful for comparison of morphology between different ammonites, even at different sizes (D), for the allometric scale factor is removed.

A MULTIDIMENSIONAL LAW OF MORPHOLOGY: THE AMMONITE "EQUATION OF STATE"

The equation is written in terms of a sub-morphospace $\mathbf{A}_1^{(4)} = \{D, U, H_1, H_2\}$ restricted to the equatorial plane of the shell:

$$U = D\left[\left(1-\frac{H_1}{D}\right)-\frac{\left(1-\frac{H_1}{D}\right)-\left(1-\frac{H_1}{D}\right)^3}{1+\left(1-\frac{H_1}{D}\right)e^{-4\left(1-\frac{H_2}{H_1}\right)\left(\frac{H_2}{H_1}\right)^{-1}}}\right] \quad \text{(equation 1)}$$

The aim of this section is to present the "equation of state" (eq. 1) and its evaluation with our data matrix, showing to the reader about its practical usage for describing the morphology of the ammonite conch. We show how it was obtained in the following chapter.

The meaning of our model is that the morphology of the ammonite in the equatorial plane is characterized by D, U, H_1 and H_2 and these dimensions are constrained each other to fit equation (1), which is then called the "equation of state". If the equation of state is meaningful, we must be able to estimate one of the dimensions involved, given the remaining ones, with close approximation to actual values. Evaluation of equation (1) was based on the 25 species studied (Table 1), on which we estimated U/D. Estimations were then evaluated by means of three different tests. Three cases have been selected to

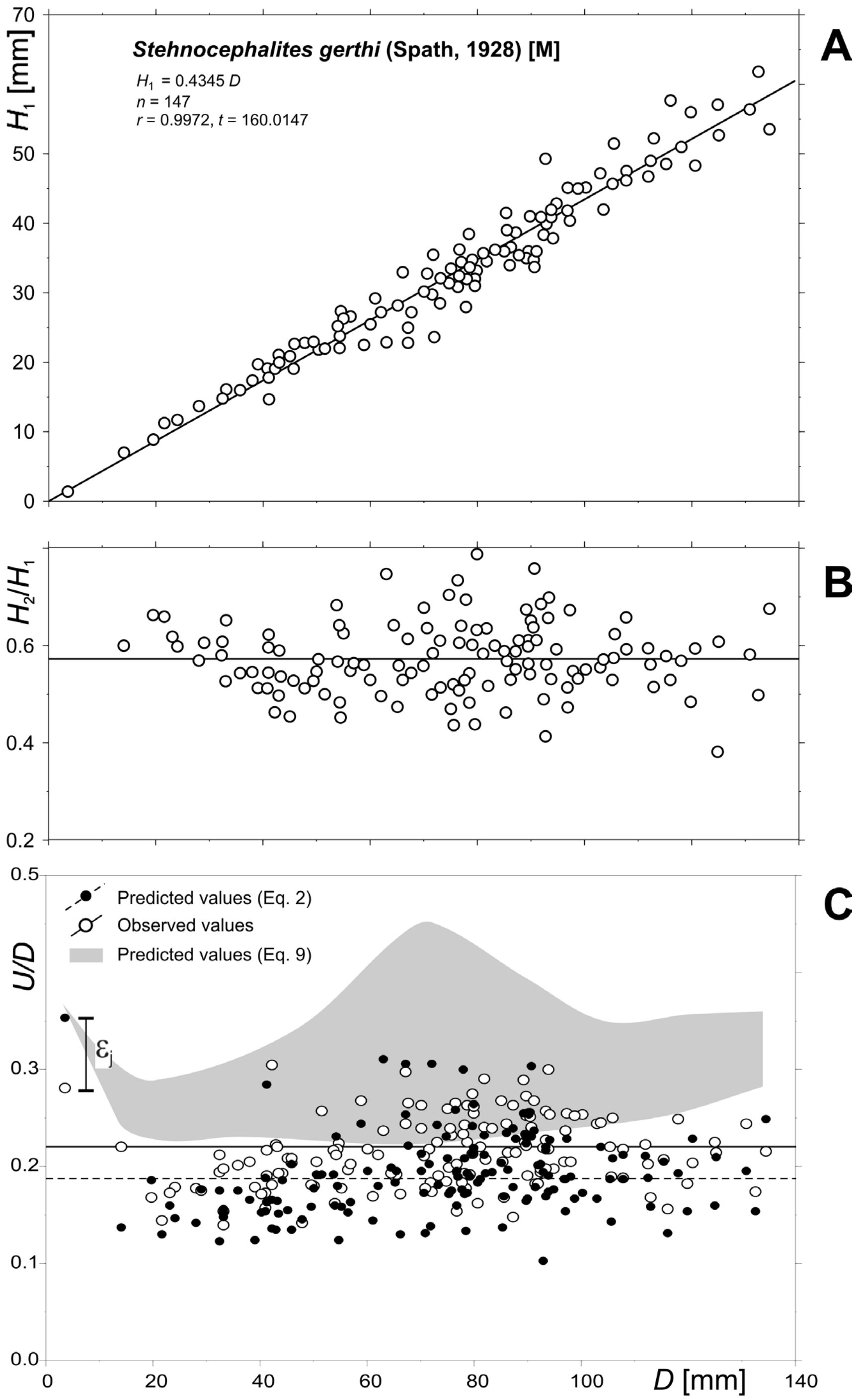

Fig. 3: *Stehnocephalites gerthi* (SPATH). A: Growth of H_1 with size (D). B: Variation of H_2/H_1 with size (D). C: Observed and predicted U/D versus D.

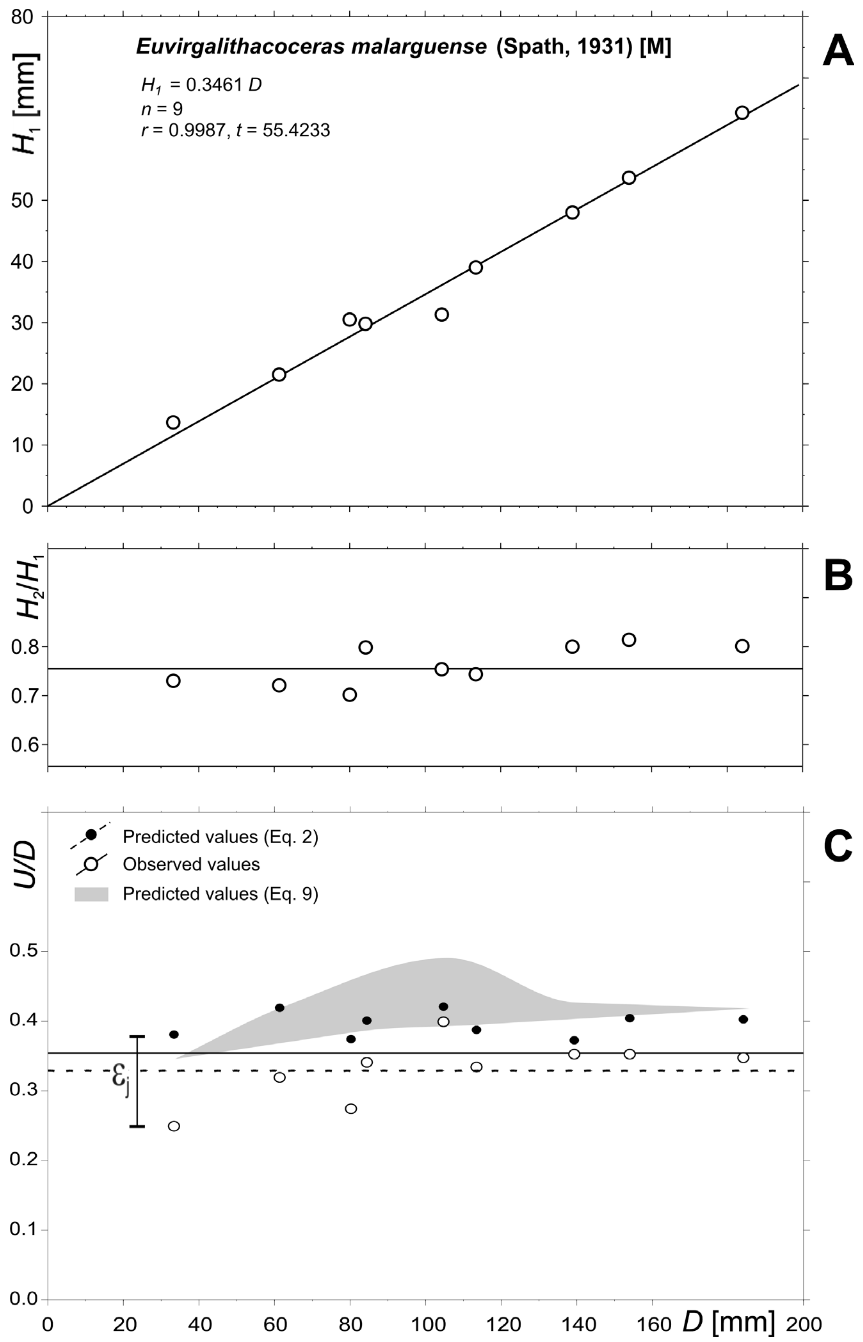

Fig. 4: *Euvirgalithacoceras malarguense* (SPATH). A: Growth of H_1 with size (D). B: Variation of H_2/H_1 with size (D). C: Observed and predicted U/D versus D.

show details of the analysis: *Stehnocephalites gerthi* (Fig. 3), *Euvirgalithacoceras malarguense* (Fig. 4), and *Pseudolissoceras zitteli* (Fig. 5).

Test 1. Figures 3A-5A show H_1 versus D for the selected species. Within all pairs of dimensions the best linearly correlated are H_1 with D. It is true in all species studied and most probably in most of the Ammonitina (*e.g.*, DAVID-HENRIET, 1962: p. 27, ATROPS, 1982, CALLOMON *et al.*, 1992, THIERRY, 1978, PARENT, 1997, 1998). The linear correlation is so high ($r > 0.9$) in regressions forced to the origin that the slope is virtually equal to the mean $\langle H_1 / D \rangle$. Figures 3B-5B show H_2/H_1 versus D, the solid line is the average value $\langle H_2 / H_1 \rangle$ around which the observed values appear to be tightly concentrated. Being that all the species studied tend to have constant H_1/D and H_2/H_1 values, we can use $\langle H_1 / D \rangle$ and $\langle H_2 / H_1 \rangle$ in the right hand of the equation (1). After this assumption the term between brackets on the right hand is a constant value called $(U/D)_{pred}$ whose magnitude depends on

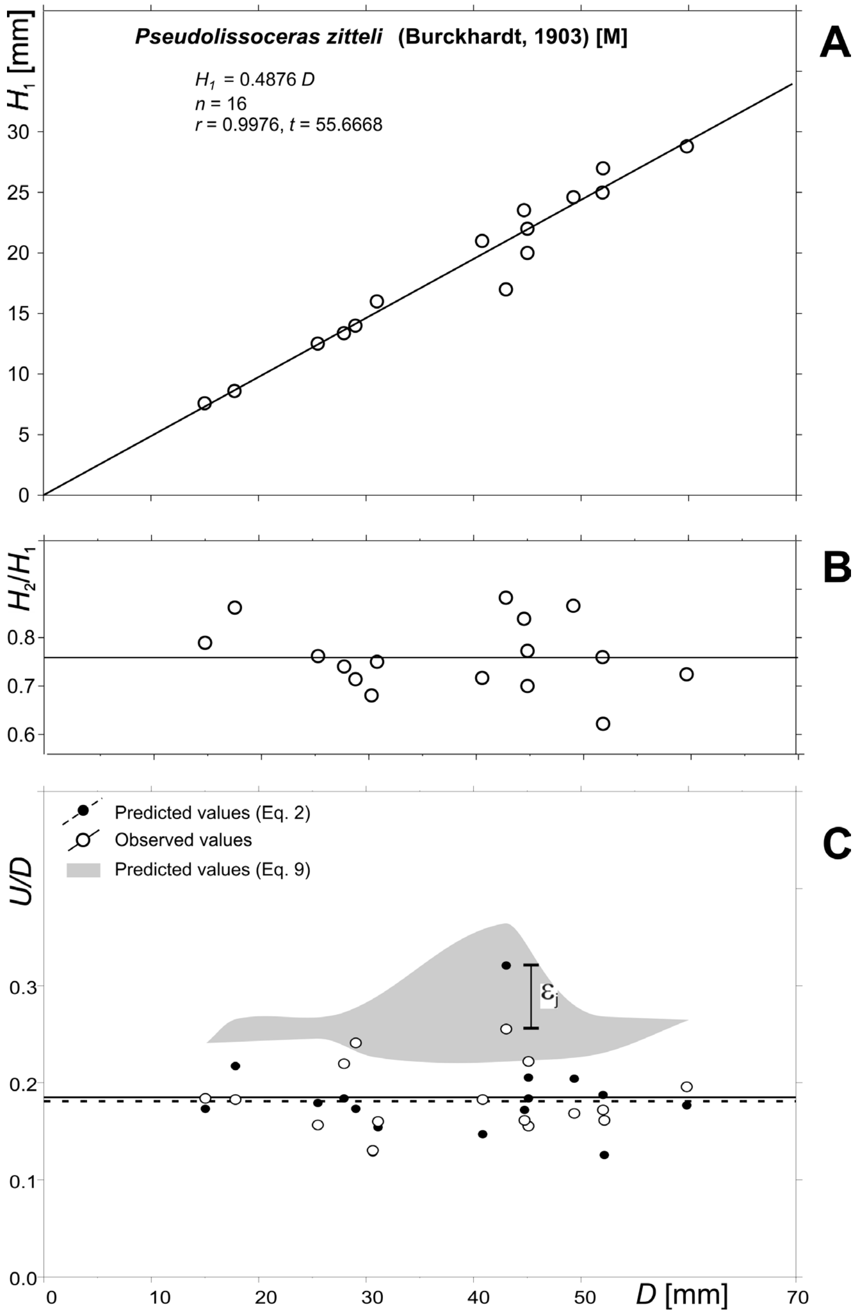

Fig. 5: *Pseudolissoceras zitteli* (BURKCHARDT). A: Growth of H_1 with size (D). B: Variation of H_2/H_1 with size (D). C: Observed and predicted U/D versus D.

the average ratios $\langle H_1/D\rangle$ and $\langle H_2/H_1\rangle$ of a given species. Therefore, we assume that U and D are linearly correlated with slope $(U/D)_{pred}$ (equation 2):

$$\left(\frac{U}{D}\right)_{pred} = \left[\left(1-\left\langle\frac{H_1}{D}\right\rangle\right) - \frac{\left(1-\left\langle\frac{H_1}{D}\right\rangle\right)-\left(1-\left\langle\frac{H_1}{D}\right\rangle\right)^3}{1+\left(1-\left\langle\frac{H_1}{D}\right\rangle\right)e^{-4\left(1-\left\langle\frac{H_2}{H_1}\right\rangle\right)\left(\left\langle\frac{H_2}{H_1}\right\rangle\right)^{-1}}}\right] \quad \text{(equation 2)}$$

In order to corroborate the validity of our analysis we have compared $(U/D)_{pred}$ (calculated following the steps described above) with the average value $\langle U/D\rangle_{obs}$ of the ratio U/D of all available measurements for each species. Columns 7 and 8 of Table 1 show the values of $\langle U/D\rangle_{obs}$ and $(U/D)_{pred}$ respectively. The first inspection of these numbers shows that they are very close. In order to better evaluate the degree of agreement, we have calculated the relative error between $\langle U/D\rangle_{obs}$ and $(U/D)_{pred}$. Table 1 (column 9) shows the percentual error of estimation as $\varepsilon(\%) = 100\left|(U/D)_{pred} - \langle U/D\rangle_{obs}\right| \langle U/D\rangle_{obs}^{-1}$, ranging from 0.7 % to 21.8 %, indicating that the “equation of state” is, from a general point of view, capturing or describing about 80-90% of the mean morphology of the ammonite conch in the equatorial plane.

In Figs. 3C-5C the ratio *U/D* versus *D* for each individual measurement of the corresponding species (observational cloud) is plotted by open circles. In these figures the solid and dashed lines represent $\langle U / D \rangle_{obs}$ and $(U / D)_{pred}$ respectively. The reader can easily note that the dashed line is inside the observational cloud and close to the solid line. It can be observed in Table 1 that $\langle U / D \rangle_{obs}$ takes values in a broad range, and, in spite of this, equation (1) can predict *U/D* with small relative errors following the ontogenetic changes.

In other words, if all the individuals of a given species have the same H_1/D and H_2/H_1 proportions (as they actually tend to do) the observational cloud given by open circles in Figs. 3C-5C will collapse in a straight line given by the predicted dashed line.

The plot of $(U / D)_{pred}$ versus $\langle U / D \rangle_{obs}$ for all the species studied (Fig. 6A) shows, as a whole, a very good correlation between predictions and observations as indicated by the tight concentration of points around the solid line $(U / D)_{pred} = \langle U / D \rangle_{obs}$. However, the first impression after looking at Fig. 6A is that the Perisphinctoidea have the larger errors of estimation. Nevertheless, the distribution of the errors of estimation $\mathcal{E}(\%)$ relative to $\langle U / D \rangle_{obs}$, with no allometric factor influencing, indicates the absence of any pattern or trend in this sense (Fig. 6B-C). The points are randomly distributed, unrelated to any particular morphotype, indicating that the "Equation of state" has no preferential bias and, as a model, is well suited for description of a large and significant part of the ammonite morphology.

Test 2. A more constraining evaluation is to apply equation (1) for individual measurements, one by one, and for each species. Therefore, for a given individual using its actual values H_1/D and H_2/H_1 we estimated *U/D*. In Figs 3C-5C we show by solid black circles the predicted *U/D* for each individual mesurement (the predicted cloud), which is plotted with the actual measurements (open circles). In the three graphs e_j shows, as an example, the deviation of a predicted value from the actual one. Column 10 of Table 1 shows the averages $\langle U / D \rangle_{cloud}$

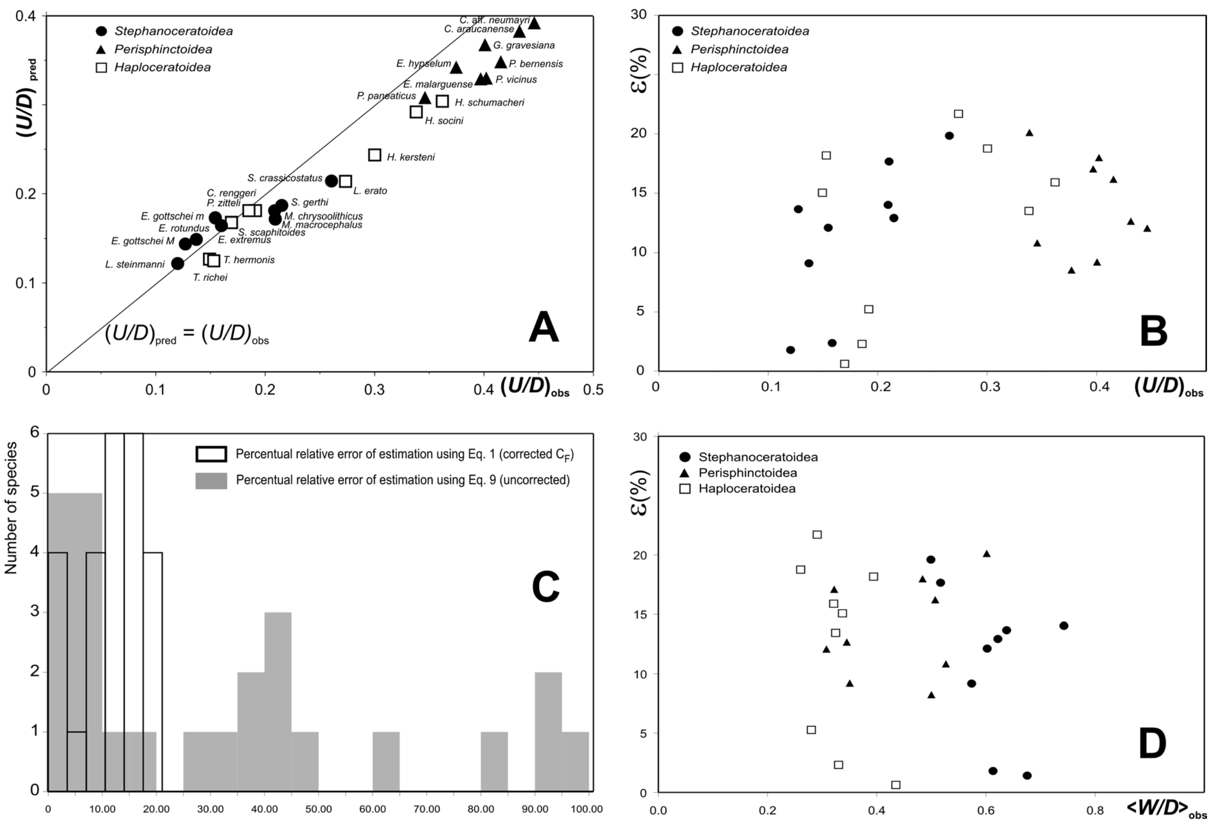

Fig. 6: A. Comparison of mean values of observed *U/D* with predicted *U/D* for all the ammonites studied. The line represents identity between observation and prediction. B: Distribution of percentual relative error of estimation of *U/D* versus mean observed values of *U/D*. C: Histograms of distribution of relative errors of estimation after prediction with and without correction factor C_F. D: Distribution of errors of estimation of *U/D* respect mean observed whorl width *W/D*.

obtained from the predicted cloud of each species, resulting always very close to $(U / D)_{pred}$.

Test 3. In order to evaluate the limits of the model (eq. 1) for describing quantitatively other coiled cephalopod shells, it was used for estimation of *U*/*D* in some Jurassic nautilids described by TINTANT *et al.* (2002). Results (Table 2) show predictions of *U*/*D* strongly biased respect the actual values. Relative errors are not only very high (ranging from 51 to 184%) but they are very heterogeneous, indicating high inestability of the equation of state for describing the relationships between dimensions in nautilids. This behaviour is originated in the growth mode of the nautilids, very different to that of the ammonites. In terms of the logarithmic spiral law (see below) on which was based our model: ρ_0 (diameter of the initial chamber) is much larger in nautilids (about 1-3 mm, LANDMAN, 1988) than in ammonites (about 0.30-0.70 mm, LANDMAN *et al.*, 1996). Therefore the number of whorls for comparable diameter is always lower in nautilids. In other words, the ratio of the diameter of the embryonic shell to that of the adult's is about 10^{-2} to 10^{-3} in ammonites but about 10^{-1} in nautilids (LANDMAN, 1988). The few cases evaluated are enough to prove that equation (1) does not represent the natutilid shell, *i.e.*, the morphospace $\mathbf{A}_1^{(4)} = \{D, U, H_1, H_2\}$ of Jurassic ammonites is different from that of the nautiloids.

From tests 1 and 2 we conclude that equation (1) efectively capturates about 80-90% of the morphology of the shell, indicating that the variables are constrained to take values fitting equation (1). The missing 10-20% could be due to fluctuations of source unknown and/or another variable not included in equation (1), such as *W*. Nevertheless, the errors of estimation ε(%)of equation (2) are uncorrelated with $(W / D)_{obs}$ as shown in Fig. 6D, where the random distribution indicates no patterns of distribution related to *W*.
In Fig. 7 each one of the species studied is represented by the pair of numbers $(\langle H_1/D\rangle, \langle H_2/H_1\rangle)$, which confidently may be considered constants as pointed out above. On the other hand, as can be seen in equation (1),

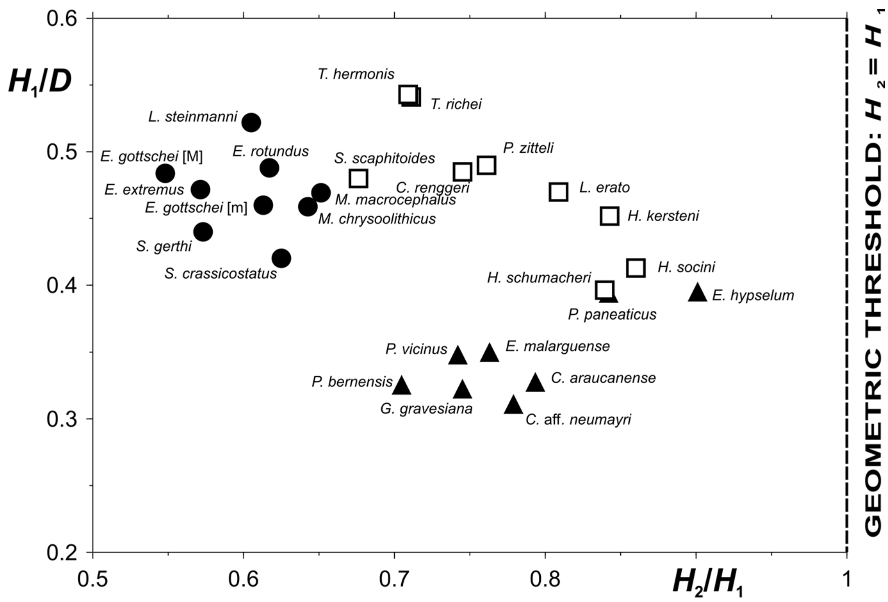

Fig. 7: Mean values of H_1/D respect to H_2/H_1 for all the ammonites studied.

Table 2: Nautilid species described by TINTANT *et al.* (2002). Measured relative dimensions and predictions of *U*/*D* based on the mean values and using equation (1). Symbols and abbreviations as explained in text. *N*: number of specimens; *n*: total number of measurements.

Species	*N*	*n*	$\langle H_1/D\rangle$	$\langle H_2/H\rangle_1$	$\langle U/D\rangle_{obs}$	$(U/D)_{pre}$	ε (%)
Pseudaganides royeri (DE LORIOL, 1872)	3	3	0.521	0.612	0.061	0.123	101.6
Pseudaganides loeschi TINTANT *et al*., 2002	1	1	0.538	0.589	0.038	0.108	184.2
Pseudaganides pulchellus TINTANT *et al*., 2002	2	2	0.642	0.596	0.109	0.053	51.4
Pseudaganides n. sp. *in* TINTANT *et al*. (2002: 434)	1	1	0.597	0.595	0.032	0.074	131.3

the term between brackets on the right hand depends on these two dimensionless quantities rather than on H_1, H_2 and D separately. There are well delimited clusters corresponding to each superfamily: the Perisphinctoidea and Stephanoceratoidea are well separated, and the Haploceratoidea is somewhat more loosely and broadly distributed between them. The variables H_1/D and H_2/H_1 are associated in such form that clusters correspond clearly to the current classification, at superfamily and family levels (*e.g.*, DONOVAN *et al.*, 1981), which was adopted for the studied ammonites before design of model and calculations (cf. Fig. 2).

DERIVATION OF THE EQUATION OF STATE. THE CONCEPT OF THE IDEAL AMMONITE

The first step was to consider an ammonite with non-ovelaping whorls, as represented in Fig. 1 (left), which grows ideally following the logarithmic law

$$\rho = \rho_0 e^{\lambda\theta} \text{ (equation 3)},$$

where ρ is the spiral radius, λ is the growth rate (assumed constant), θ is the spiral angle (*e.g.*, $\theta = \pi$ = half-whorl) and ρ_0 is the initial radio or protoconch diameter. Following this simple model (Fig. 1, left side):

$$D = \rho_1 + \rho_1' = \rho_0\left[e^{\lambda\theta_F} + e^{\lambda(\theta_F - \pi)}\right] \text{ (equation 4), and}$$

$$H = \rho_0\left[e^{\lambda\theta_F} - e^{\lambda(\theta_F - 2\pi)}\right] \text{ (equation 5),}$$

where θ_F is the final angle or number of whorls. Using the expression for H and D we have:

$$H / D = (1 - e^{-2\lambda\pi})\,(1 + e^{-\lambda\pi})^{-1} \text{ (equation 6)}$$

which indeed is a constant as mentioned above, and being relevant for the subsequent analysis. This equation does not include any of the quantities: spiral radius, number of whorls and protoconch diameter. Growth rate may be written:

$$\lambda = -\frac{1}{\pi}\ln\left(1 - \frac{H}{D}\right) \text{ (equation 7).}$$

Then from Fig. 1, we have $U = D - H - H'$. Thus writing H' in terms of the logarithmic law and using equation (7) for λ we obtain the following relationship for the non-overlapping whorls ammonite:

$$U = D\left[\left(1 - \frac{H}{D}\right) - \frac{\left(1 - \frac{H}{D}\right) - \left(1 - \frac{H}{D}\right)^3}{1 + \left(1 - \frac{H}{D}\right)}\right] \text{ (equation 8).}$$

H is the distance between points p_0 and p_1 in the ideal ammonite of Fig. 1 (left side), thus the equivalent of H in the real ammonite (Fig. 1, rigth side) should be H_2. Nevertheless, for satisfying the condition $U = D - H - H'$ it must be used H_1 for obtainig $U = D - H - H_1'$, and equation (8) is transformed into

$$U = D\left[\left(1 - \frac{H_1}{D}\right) - \frac{\left(1 - \frac{H_1}{D}\right) - \left(1 - \frac{H_1}{D}\right)^3}{1 + \left(1 - \frac{H_1}{D}\right)}\right] = D\left(1 - \frac{H_1}{D}\right)^2 \text{ (equation 9)}$$

The difference between the coiling of the real ammonite with respect to the logarithmic spiral model is that whorls of the former overlap one another, thus the distance between p_0 and p_1 becomes smaller. Consequently the umbilicus (U) and diameter (D) become smaller too (see Fig. 1).

After testing equation (9) with our data matrix by means of prediction of U/D we immediately noted that this is not enough accurate and homogeneous (stable) in predicting. Last column of Table 1 shows the percentual error $\varepsilon'(\%)$, between observations and predictions from equation (9). A simple inspection on these numbers shows that errors are very heterogeneous and running from small values of the order of 0.1 % (*Hecticoceras kersteni*) to very large values of the order of 100% (*Eurycephalites gottschei*). In all cases where large errors are produced, U was overestimated. Figures 3C and 5C show, by a shaded area, the region where the predicted values for U/D are located when they are estimated using equation (9). Clearly, the shaded areas are only slightly overlapped with the observed cloud, indicating overestimation of U/D. Note that this is not the case for *Euvirgalithacoceras malarguense* (Fig. 4C) where the shaded area is partially overlapped by the observed cloud in a consistent way with the low error $\varepsilon'(\%)$ of about 5%.

The percentual errors $\varepsilon'(\%)$ for the Stephanoceratoidea are all systematically large while those for the Perisphinctoidea are all systematically low (Table 1). On the other hand H_2/H_1 is larger in Perisphinctoidea than in Stephanoceratoidea (Fig. 7). Therefore, it is evident that the source of the large $\varepsilon'(\%)$ in Stephanoceratoidea is originated in the preliminary assumption of null-overlap ($H = H_2 = H_1$) of the ammonite model used (Fig. 1, left side), whereas the ammonites of interest (Fig. 1, right side) have a clearly evident and variable overlap ($H_2 < H_1$). As Peripshinctoidea has H_2/H_1 closer to one, equation (9) gives better results in these superfamilies.

Following phenomenological arguments based on the discussed observations we included a correcting factor C_F in the denominator of the third term of equation (9) obtaining equation (1). This correcting factor must be H_2/H_1-dependent in order to take into account the above observed pattern. We have evaluated several forms for C_F, finding that an appropriate one is $C_F = e^{-4(1 - H_2 H_1^{-1})(H_2 H_1^{-1})}$. This corrective factor can be written as $C_F = e^{-4(H_1 - H_2)H_2^{-1}}$, in the form of another measurement of involution. It is important to note that inclusion of this correcting factor leads to the reduction and homogenization of all predictions as shown by the even distribution of values of $\varepsilon(\%)$ (Fig. 6C), restricting them in within a range of 1-22% (cf. Table 1). This regularization allows to treat all species on equal footing.

Another form for equation (1) is:

$$U = D\left(1-\frac{H_1}{D}\right)^2\left[\frac{C_F+\left(1-\frac{H_1}{D}\right)}{1+C_F\left(1-\frac{H_1}{D}\right)}\right] \quad \text{(equation 10)}$$

which shows the third factor, on the second hand sign, as a correction to the second one in order to approximate the ideal ammonite to that with overlapping of its whorls, that is $H_1 > H_2$.

In the Haploceratoidea, differently to Perisphinctoidea and Stephanoceratoidea, the errors $\varepsilon'(\%)$ are very heterogeneous. As can be seen in Fig. 7, Perisphinctoidea and Stephanoceratoidea form well separated clusters in the plane (H_2/H_1, H_1/D) while Haploceratoidea is widely distributed between both groups. In agreement with this pattern, the percentual errors $\varepsilon'(\%)$ obtained with equation (9) are also heterogeneous in contrast to Perisphinctoidea and Stephanoceratoidea. The open squares in Fig. 7 with large $\varepsilon'(\%)$ tend to be close to Stephanoceratoidea which also has large $\varepsilon'(\%)$. On the other hand, open squares with small $\varepsilon'(\%)$ tend to be close to Perisphinctoidea which also have small $\varepsilon'(\%)$. The meaning of these patterns is that equation (9), which describes the ideal amonite with non-overlapping whorls, does not make a clear distinction of Haploceratoidea from the other superfamilies.

Equation (1) is robust and captures, with less than 20% of uncertainty, the morphology of completely different ammonites. In this sense the main contributions of this modelization are: (1) the translation of the old discussion about the logarithmic spiral growth to a language in terms of the clearly measurable variables H_1, U and D in the form of equation (9); (2) the inclusion of a H_2/H_1-dependent correcting factor C_F fulfils the gap between the ideal ammonite described by equation (9) and the real ammonite described by equation (1); and (3) as a corollary, another interesting consequence is that from equation (7) may be derived the so called "whorl expansion rate" (*WER*, KORN, 2000):

$$e^{2\pi\lambda} = \left(\frac{D}{D-H_2}\right)^2 = \left(\frac{D_n}{D_{n-1}}\right)^2,$$

where n is whorl number (cf. CALLOMON *et al.*, 1992 for the last term).

The dimension which controls or regulates the growth in $\mathbf{A}_1^{(4)} = \{D, U, H_1, H_2\}$ is hard to identificate. During the initial part of our research we have not made any a-priori assumption on this matter. Prima-facie, H_2, direct representative of the growth rate (see equation 7), seems to be the natural candidate. Nevertheless accounting for results obtained and for the greatest developmental stability of H_1 (better than canalization suggested in PARENT, 1998), both during the ontogenetic development and as intraspecific variation, we believe that H_1 is the most constraining dimension of the post-embryonic ammonite growth. The control exerted by H_1 on shell morphogenesis seems to go beyond the external shell geometry; a direct relationship between sutural complexity (measured as fractal dimension) and whorl height was statistically demonstrated by OLÓRIZ *et al.* (2002: 161). On the other hand it is clear that H_2/D is a measure of the relative growth rate of shell diameter, and H_2/H_1 is a measure of involution not ambiguous as the currently used *U/D*. After comprobation of the importance of H_2 for characterization of the ammonite shell, we take the opportunity to suggest the measurement of this dimension whenever possible.

CONCLUSION

We have worked with three "ammonites": (1) the real or actual ammonite (our target with $H_2 < H_1$); (2) an intermediate figure: the non-overlapping whorls or ideal ammonite ($H_1 = H_2$) described by equation (8); and (3) the theoretical ammonite, that is, an approximation to the real ammonite by means of the equation of state (equation 1). The equation of the intermediate, or ideal, ammonite ($H_1 = H_2$) should be the equation of state for a large group of Jurassic (and possibly Cretaceous) ammonites whose whorls do not overlap. It opens another line of research, similar to the presented here, beginning with the evaluation of equation (1) for predicting those types of ammonites.

Working to write the log spiral law in terms of the variables most commonly used to describe the morphology of ammonites, it was obtained, at first, equation (9) written in terms of *U, D* and H_1. This equation which we called "equation of state for the ideal ammonite" leads to very large and heterogeneous errors, between predictions and observations of *U/D*, running from 1 to 100%. The source for these errors lies on the fact that the ideal ammonite has null-overlap while the real ammonite shows clear overlapping in its whorls expressed through the relation $H_2 < H_1$. Introducing into equation (9) a corrective factor in the form of a measure of the overlap of whorls (H_2/H_1) we arrived to the proposed "equation of state of the real ammonite". Applying this model on our samples from 25 species relative errors become homogeneously distributed and relatively small, running from 1% to 20%. We interpret these results in the sense that equation (1) capturates 80-90% of the morphogenetic relationships between dimensions in the morphospace $\mathbf{A}_1^{(4)}$, at least for Middle and Upper Jurassic ammonites. In this form the gap between the mathematical description of the ammonite shells with overlapping and non-overlapping whorls is mostly fulfilled.

The width of whorl section (*W*) is not associated in direct or explicit form with the development in the equatorial plane, which is in accord with the characteristically wide intraspecific variation of W/D seen in most ammonoids. It is important to note that the main variables involved in equation (1) are the dimensionless quantities H_1/D and H_2/H_1 and that the mean values of these two quantities, for each species, correlate forming well delimited clusters for each superfamily (Fig. 7). It is concluded that H_1/D and H_2/H_1 keep relevant information of the corresponding species and superfamily and can be considered as fundamental parametres to describe the basic form of ammonites.

Application of equation (1) into Jurassic nautilids produces estimations with large and heterogeneously distributed errors, in accord with the different growth mode of nautilids with respect to ammonites. It is well known that *Nautilus* is a poor model for comparative morpho-functional studies on ammonites (see JAKOBS & LANDMAN, 1993) ; results presented in present paper give additional support, from an independent line of evidence, to this fact.

As a final reflection it is interesting to point out some analogies between the present study and others in physics which have given us inspiration at the beginning of this work. In thermodynamics it is well known that the state of a given gas is characterized by the relevant variables T (temperature), P (pressure) and V (volume). These are not free to take any value. They are always connected by an equation of state. The most known is the equation of state for the ideal gas : $PV = n\mathrm{R}T$, where n is the number of moles and R is the constant of gases (see, e.g, KAUZMANN, 1966). This is, of course, not an exact expression but without doubts captures a relevant behaviour of the system. How the gas arrives to a given state is not relevant for thermodynamics but in this state the equation of state is fulfilled. Much time passed until researchers undestood the role of molecules in the behaviour of gases. For instance, it is well known that the macroscopic constant R can be expressed in terms of the Boltzman constant k_B and the Avogadro number N_A ($R = k_B N_A$), both having a clear atomic meaning. It may be, that in biology something similar can be expected. May it be that in the future, biologists can describe the phenotype in terms of genes as physicists describe the gases in terms of molecules? However, what was always clear in physics is that, before understanding the role of molecules it was relevant to have a very clear picture at a macroscopic level. That is, the deep knowledge of the equation of state. We hope our work will contribute as regards this. Most of the time, people consider Physics as an exact science ; this is, in our opinion, a naïve approach. This is mainly inspired by the reduccionist conception that if we know the law of the parts we will know the law of everything. We share the opinion of ANDERSON (1972) that "more is different" in the sense that there are emergent laws and properties at every different level of organization (see also LAUGHLIN & PINES, 2000 ; LAUGHLIN *et al*., 2000). The reduccionist conception leads to think that Physics can describe the reality in an exact form. We reject this idea and point out that Physics, as an experimental science, capturates some behaviour of the system and not the whole reality. For instance, two different gases can obey the same equation of state but they can have completely different magnetic properties. Thus if we wish to describe all properties at the same time we will arrive probably to a problem whose degree of complexity will be of high order, like in biological systems. These concepts are important for understanding what we mean by "an equation of state for the (postembryonic) ammonite shell". Indeed, we hope to have capturated some regular behaviour of the ammonite morphology.

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