Advances and challenges in geotectonic modelling

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Key-words. - Numerical modelling, Rifting, Passive margins, Subduction, Orogeny, Metamorphism, Rheology

Abstract. – Thermo-mechanical numerical modelling becomes a universal tool for studying short- and long-term lithosphere processes, validating and verifying geodynamic and geological concepts and putting stronger constraints on the observational data. State-of-the-art models account for rheological and mineralogical structure of the lithosphere, implement high resolution calculations, and their outputs can be directly matched with the geological and geophysical observations. Challenges of these models are vast including understanding of the behavior of complex geological systems and processes, parameterization of rheological parameters and other rock properties for geological conditions, not forgetting a large number of future methodological breakthroughs such as the development of ultra-high resolution 3D models coupled with thermodynamic processes, fluid circulation and surface processes. We here discuss both geological and geodynamic applications of the models, their principles, and the results of regional modelling studies focused on rifting, convergent and transform plate boundaries.

Modélisation géotectonique : avancées et challenges

Mots-clés. - Modélisation numérique, Rifting, Marges passives, Subduction, Orogenèse, Métamorphisme, Rhéologie

Résumé. – La modélisation numérique thermo-mécanique devient un outil universel pour étudier les processus lithosphériques court-terme et long-terme, pour valider les concepts géologiques et géodynamiques et pour apporter des contraintes plus importantes sures, et guider, les observations. Les modèles rendent compte de la structure rhéologique et minéralogique de la lithosphère, complètent les calculs à haute résolution et leurs « outputs » peuvent être directement confrontés et ajustés aux observations géologiques et géophysiques. Les défis de ces modèles sont étendus, incluant notamment la compréhension du fonctionnement des systèmes et processus géologiques complexes, la paramétrisation des variables rhéologiques et des autres propriétés des roches selon les conditions géologiques, sans oublier bon nombre d'avancées méthodologiques futures comme le développement de modèles 3D à très haute résolution couplés aux processus thermodynamiques, aux circulations de fluides et aux processus de surface. Nous discutons dans cet article à la fois des applications géologiques et géodynamiques des modèles, de leurs principes et des résultats de modélisations plus thématiques focalisées sur le rifting et les limites de plaques convergentes et transformantes.

INTRODUCTION

Physical models (fig. 1) replace real objects when direct study presents significant complications. In many cases direct study is simply impossible due to extreme spatial and time scales, inaccessibility or complex non-linear character of the underlying phenomena. In other cases it presents substantial risks and/or technical difficulties requiring important investments in terms of time, manpower and equipment. All of these conditions apply to geodynamic and tectonic processes that occur at temporal and spatial scales largely exceeding human time scales, refer to strongly non-linear complex processes while their study often requires significant financial investments and manpower.

The history of tectonic modelling is Earth Sciences comes back to the 19 century when Sir J. Hall has designed his first analogue models explaining folding of sedimentary layers. Even if not properly scaled, these models have played an essential role in sedimentary and structural geology providing new understanding of the evolution and mechanics of the stratified lithologies. This has been very soon recognized by contemporary geologists, e.g. by one of the fathers of modern geology, Charles Lyell, in his famous "Principles of Geology" [1865, first published in 1830] and "Elements of Geology" [1862]. The first analog mechanical models correctly scaled to nature [Cadell, 1890] have appeared at the end of 19th century. Since that, mechanical models were widely used and largely contributed to our understanding of the mechanics and physics of geological and tectonic processes such as formation of rifted basins [e.g., Allemand and Brun, 1991; Brun, 1999], oceanic spreading, mantle convection, lithosphere folding, subduction and collision [e.g., Davy and Cobbold, 1980; Chemenda et al., 1996]. Analog models have a number of important

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FIG. 1. – A flow chart of a typical research study in Earth Sciences. Models play a specific role since the observations generally cannot be entirely trusted nor directly interpreted in terms of large spatial and time scale evolution. The models serve not only for prediction and reconstruction of the geological or geodynamic evolution and understanding of the governing mechanisms of the geodynamic processes but also for integration and validation of the observational data, for example, by showing that some of these data imply inconsistent evolution of the targeted process. Model predictions next serve to target new field observations.

advantages, for example, being naturally three-dimensional and efficient, in terms of time needed to fulfill series of similar 3D experiments once the experimental procedure is established (though one should mention that any new type of an analog experiment often requires building a specific experimental setting, tuning and validation of an experimental procedure that may take several months). However, growing understanding of the importance of complex rheological properties and of thermo-mechanical interactions that are difficult to implement in analog models with sufficient respect of scaling laws, has put forward numerical models (fig. 2), that, with further increase of the computing power, progressively become a dominant modelling tool. An important feature of the numerical models is also their portability, i.e. same model can be run on standard computers at different places, while analog laboratories need heavy custom equipment. Nevertheless, as well pointed out by Gerya [2011], the numerical geodynamic modelling is still a very young developing domain, if one recalls that the first numerical modelling study has been published only in 1970 by Minear and Toksöz [1970].

In the early 70ties of 20th century it has become evident (see historical overview in, e.g, Burov [2011]) that the geological "substratum" has very specific properties being able to be both viscous (fluid-like, irreversible strain without localization), elastic (i.e. reversible strain) and brittle (localized irreversible strain) depending on pressure, temperature and timescale of deformation. For example, the Earth's mantle is elastic at human timescales but is viscous on geological timescales (> 10 000 years, post-glacial rebound) and can be strongly irreversibly deformed due to solid state creep. Understanding such multi-scale interlinked processes requires integral approach. For these reasons, geodynamic numeric modelling, which has the power of combining different inter-independent physical processes, has been developing very rapidly since the past 30 years both, in terms of the number of various applications, and in terms of the numerical techniques. Geodynamic modelling stands now as one of the most dynamic and advanced fields of the Earth Sciences [Gerya, 2011].

The role of models in Earth Sciences is more versatile than in "human-scale" sciences such as engineering or biology, not only because of the impossibility of direct experiments, but also because in the Earth Sciences, the models have a wide spectra of specific functions such as verification and validation of the observational and experimental data (fig. 1). Indeed, geological observations are subject to large uncertainties being often extrapolations from local and small-time scale observations to larger spatial and temporal scales [Burov and Watts, 2006; Burov, 2011]. In difference from data of, for example, physical experiments, these observations cannot be always fully trusted since the raw data undergo important modifications and extrapolations before their application to geological problems. One of the typical examples of such modifications refers to the data of experimental rock mechanics, because the rocks are deformed under laboratory conditions that are highly different from natural conditions. Their applicability to geological conditions hence needs validation, and this function is largely fulfilled by geodynamic models that can test whether the inferred mechanical properties yield geologically-consistent behaviors at large time and temporal scales [Burov et al., 1999; Burov, 2011]. It is also noteworthy that



FIG. 2. – Comparison of analog and numerical mechanical models (courtesy of L. Le Pourhiet, modified). Both approaches are complementary and have their respective up- and down-sides. Since recent time, numerical models have been put forward due they better match for the crucial task of incorporation of multi-physical processes (thermo-mechanical coupling in the first run) and complex material properties.

due to the complexity and multi-process dependencies in geodynamic systems, simple "intuitive" hypothesis about their functioning often do not hold. One of the recent examples refers to new understanding of the mechanisms of formation of oceanic transform faults that stemos from the results of the numerical modelling [Gerya, 2010]. Despite common ideas, the numerical modelling experiments show that transform faults represent actively developing growth structures resulting from the mechanical instabilities at spreading centers, and not conventional faults, i.e. "passive" mechanical ruptures of the lithosphere. Earlier Cloetingh et al. [1999] have shown, on the base of self-consistent numerical models, and against common intuition, that lithospheric faulting does not prevent but enhances lithospheric folding, and vice-versa. Another contra-intuitive finding based on model-derived knowledge refers to later commonly accepted idea that fluids play a key role in the initialization of oceanic subduction and are responsible for subduction asymmetry [Faccenda et al., 2009]. None of these fundamental geodynamic findings could be done solely on the basis of observations or analytical considerations. The list of fundamental geodynamic and tectonic discoveries that could not be even envisaged without thermo-mechanical modelling is long and continues growing, as the models start to account more and more accurately for physical processes and multi-disciplinary observational data.

The role of modern geodynamic models is therefore is multifold-fold: (1) understanding complex processes that cannot be assessed through analytical considerations, (2) validation, via refutation, of geological and geodynamic hypothesis, (3) validation of extrapolations from observations and experimental data, (4) orienting data acquisition, new laboratory and field research through demonstrating potential sensitivities of complex processes to particular observations.

In the next sections we discuss the main features of the numerical thermo-mechanical models used in geotectonic modelling. We will then confer applications of the geodynamic models to:

- convergent processes such as subduction (simple shear), lithosphere folding and pure-shear collision (fig. 3),

- extensional processes such as active and passive rifting (fig. 3),

- lithospheric flexure and regional isostasy,
- mantle-lithosphere interactions,
- surface-tectonics interactions.

NUMERICAL MODELS OF GEOTECTONIC PROCESSES: BASIC PROCESSES

Numerical models of geological processes are based on discrete presentation of physical laws controlling the geological phenomena (fig. 4). Therefore they treat problems of tectonic and geological deformation as that of deformation of the mechanical continuum where the basic physical laws such as conservation of momentum, mass and energy are observed. These basic laws are combined with laws that describe physical properties of the system, in the first order with the constitutive equations that describe rheological properties of the rocks, with the state equations that describe changes in physical properties of rocks as function of pressure and temperature, and with the equations describing surface processes, i.e. re-distribution of surface loads due to erosion and sedimentation. Additional physical processes



FIG. 3. – Possible collision and extension scenarios where horizontal shortening or extension is accommodated or largely influenced by: (A) removal of hot mantle lithosphere by Rayleigh-Taylor gravitational instability at the bottom of mantle lithosphere, combined with pure or simple shear deformation in the crust; (B) stable pure shear accommodation (stable collision without subduction or McKenzie's [1978] rifting concept); (C) unstable mode due to tensional or compressional instabilities (folding or boudinage); (D) stable uniform simple shear mode (subduction or rifting according to Wernicke's [1985] concept). Related large-scale parameters characterising collision style, lithospheric strength and rheology: $T_{e,r}$, F, σ, u , De, τ_m , h, L, λ, ϕ, T_e is equivalent elastic thickness. F, σ, u are respectively the horizontal force, stress and convergence/extension velocity, that are linked to the lithospheric strength and possible deformation related to the thickness of the competent layers in the lithosphere. h, L are respectively the vertical and horizontal scale for process-induced topography supported by lithospheric strength, Argand number Ar = pghL/F. ϕ is subduction or major thrust fault angle that is indicative of the brittle properties and of the overall plate strength.

are also often plugged-in such as fluid flow and melting [e.g., Faccenda *et al.*, 2009; Angiboust *et al.*, 2012].

The momentum equation corresponds to the Newton's second law of motion and describes the *conservation of momentum* for a continuous medium in the presence of gravity forces:



FIG. 4. – Flow chart of multi-physical processes considered in the numerical models (modified after courtesy of M. Billen) .

$$\frac{D\dot{u}_i}{Dt} = \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_i} + g_i \tag{1}$$

where D/Dt corresponds to objective derivative (in the Lagrangean framework), u is displacement, \dot{u}_i are velocity components (i.e., time derivatives of displacement), ρ is density, σ_i is stress tensor components, x_j are coordinate components and g_i are acceleration due to gravity components.

Stresses are related to strains $\varepsilon (= \int \dot{u} dt)$ and strain rates $\dot{\varepsilon} (= \nabla \dot{u})$ via constitutive equations that may take various forms depending on rock rheology:

$$\frac{D\sigma}{Dt} = F(\varepsilon, \dot{\varepsilon}, \sigma, T, \dots) = F(\dot{u}, \nabla \dot{u}, \sigma, T, \dots)$$
(2)

where T is temperature that contributes to buoyancy and plays essential role in case of ductile rheologies, as well as in case of rheological changes due to metamorphic reactions. Due to the temperature dependence of body forces and rheological properties, and, hence, of stresses, as well as due to the fact that constraining the thermal evolution of the system is important by itself, (1) and (2) have to be coupled with the heat transfer equation:

$$\frac{DT}{Dt} = \frac{1}{\rho C_p} \nabla(kT) + \sum_{i=1}^n H_i$$
(3)

where k, C_p, T, H_i designate respectively thermal conductivity, specific heat, and internal heat production per

unit volume coming from different sources (*i* designates head-producing source, e.g. radiogenic heating or frictional heating).

Equations (1-3) constitute a starting base of all present-day mechanical numerical models of geodynamic and geological processes. In simplest case, only single rheology type is taken into account (eq. 2), for example viscous, plastic or elastic. In most advanced models, constitutive equations (2) account for complex viscous-elastic-plastic rheologies that characterize real rocks [e.g., Burov and Yamato, 2008; Gerya, 2010]. Depending on the degree of the realism of the models, heat transfer equation (3) may take into account different kinds of internal heat sources such as radiogenic heat production, frictional heating, latent heating, and so on.

Since density affects body forces and heat transfer, its variations must be also taken into account, which is reflected with different degrees of sophistication by state equations:

$$\rho = f(P, T) \tag{4}$$

The simplest form of these equations accounts only for thermal expansion (called simple Boussinesq approximation). More advanced approaches consider density and rheological variations associated with phase transforms on the basis of thermodynamic petrology models such as the program set Perple_X [Conolly, 2005]. This directly links the equation (4) with the equation (2). In continental domain, surface topography is actively modified by surface processes, whose rates in actively deforming zones are nearly the same as the rock uplift rates [e.g., Avouac and Burov, 1996]. Hence, surface processes models need to be also included, which is generally done in the following form [Culling, 1960]:

$$\frac{Dh}{Dt} = f(h, \nabla h, \nabla h, k_{err}, ...)$$
(5)

Where *h* is surface topography elevation, $k_{\rm err}$ is surface erosion coefficient, and the other parameters (not shown here) may include river discharge and dip, geometrical characteristics of the fluvial network, precipitation, climate conditions and so on [e.g., Willet, 1999]. In most simple cases, simple diffusion of topography with coefficient $k_{\rm err}$ is used to simulate surface processes [e.g., Avouac and Burov, 1996; Burov and Toussaint, 2007].

Finally, it has recently become clear that fluids may play a very important role in localization of deformation in various geodynamic contexts. For example, it has been shown that they may play a major role in subduction processes [Faccenda *et al.*, 2009; Angiboust *et al.*, 2012]. Hence, fluid circulation and partial melting have to be taken into account with different degree of physical and observational consistency in most cases [Gerya, 2011]. The simplest models [Arcay *et al.*, 2007] impose fluid migration in predefined (basically vertical) direction, more realistic models implement Darcy's porous flow or even more complete bi-phase flow formulations [e.g. Mezri *et al.*, 2013].

CONVERGENT PROCESSES

There is no surprise that the first numerical geodynamic models addressed mechanisms of oceanic subduction [Minear and Toksoz, 1970] and of mantle convection [Torrance and Turcotte, 1971], as two key processes behind

- that time newly-born - plate tectonics theory. In both cases the role of thermal advection is essential and could not be consistently handled by analog models justifying numerical approach. The models of continental collision have followed the oceanic subduction models few years later [Daignières et al., 1978; Bird, 1978]. Since that, numerical models have been widely used for understanding various aspects of the convergent processes. A large number of studies have been focused on the oceanic subduction and have demonstrated that simple analytical models of sea-floor spreading and even numerical convection models that treat the lithosphere in simplified way, fail to explain some key observations associated with subduction. According to the plate tectonics theory, plates sink into the mantle when they become old and cold and hence negatively buoyant. Despite the elegant simplicity of this idea, it has met a number of major consistency problems when flexural observations and model have shown [Cloetingh et al., 1982; Watts, 2001] that plate strength grows with age so that old plates are so strong that they cannot bent down and hence cannot subduct. Furthermore, it has been also demonstrated that friction in the subduction channel would also strongly prevent subduction processes unless some mechanism of lubrication is not activated [Hassani et al., 1997]. The other enigmatic problem refers to the fact that the oceanic subduction is one-sided, while, from general point of view, both colliding plates should subduct symmetrically together. 30 years of numerical thermo-mechanical modelling has been required to show that plate flexure, or bending, initiates localized weakening of the brittle-elastic-ductile lithosphere [e.g., Burov and Diament, 1995; Burov, 2010] (fig. 5) and that fluids penetrating into the fractures networks created by flexural yielding result in further weakening of the plate enabling oceanic subduction [Faccenda et al., 2009] (fig. 6, 7). This mechanism also explains the mechanism of one-sided subduction, e.g. why only one of the converging oceanic plates subducts below the other. The next contra-intuitive problem related to oceanic subduction and successfully assessed by numerical modelling refers to the processes leading to slab-break-off and to the impact of slab breakoff on the surface evolution and on the following subduction history, including continental collision. It has been shown [Duretz et al., 2011] (fig. 8) that timing and depth of the slab-break-off are conditioned by multiple factors and that topographic impact of the slab-break off is a strong function of the slab-break-off depth, subduction rate, plate rheology and thermal age. 3D modelling studies of subduction processes made significantly evolve our vision of subduction dynamics by showing that subduction can be strongly affected by out-of plane flow so that slab-break-off can be initialized as a progressive out-of-plane tear of the slab (fig. 9) [Burkett and Billen, 2010; Stegman et al., 2010]. Hence, simple initial ideas on the mechanisms of oceanic subduction are conditioned by very complex processes, which at the end provide new elements for explanation of the uniqueness of the terrestrial plate tectonics.

While subduction is a predominant mechanism to accommodate plate convergence in the oceanic realm, except few zones of oceanic folding in Indian Ocean [e.g. Gerbault *et al.*, 1999], in continents it is only the one of four possible ways of accommodation of shortening (fig. 3): pure-shear (i.e. volumetric thickening); stable subduction (or underplating), which is simple shear sliding of one plate below



FIG. 5. – Models [Burov and Diament, 1995] predicted that flexural weakening is one of the primary mechanisms explaining bending of strong cold plates prior to subduction. Flexural strain are proportional to local plate curvature and increase with the distance from the neutral plane. Hence, the associated brittle and ductile stresses may locally reach yield limits resulting in localized weakening due to faulting at the surface and ductile weakening at the base of the plate.

the other; folding [Burg and Podladchikov, 2000; Cloetingh et al., 1999]; instable pure or simple shear shortening, also dubbed "unstable subduction" and related to the development of gravitational Raleigh-Taylor instabilities in thickened, negatively buoyant lithosphere [e.g., Houseman and Molnar, 1997]. All these scenarios can be superimposed in nature. For instance, "megabuckles" created by lithospheric folding [Burg and Podladchikov, 2000] may (at least in principle) localize and evolve into subduction-like thrust zones or result in the development of Rayleigh-Taylor instabilities. On the other hand, RT and boudinage instabilities may occur in subducting slab leading in its break-off when it loses initial mechanical strength due to conductive heating from the surrounding mantle [Pysklywec et al., 2000]. This complexity and diversity of convergence mechanisms in continental domain has been well demonstrated by the numerical experiments [e.g., Toussaint et al., 2004; Burov

and Yamato, 2008; Sizova et al., 2010]. Indeed, due to overall positive buoyancy of the continental lithosphere, some very special conditions must be created to enable continental subduction [e.g., Cloos, 1993; Afonso and Zlotnik, 2011], otherwise the lithosphere would accommodate shortening in a different way. Nevertheless, the presence of exhumed UHP rocks, seismic tomography, structural and mass balance studies indicate that continental subduction should take place in a number of cases such is European Alps or Himalayan collision [e.g., Burov et al., 2001; Toussaint et al., 2004a, 2004b; Ford et al., 2006; Yamato et al., 2008; Zhang et al., 2009; Handy et al., 2010; Tetsuzo and Rehman, 2011]. Moreover, some of these studies show, on the basis of petrological evidence, that not only dense mantle and relatively dense lower crust but also an essential part of the upper crust and sediment can be buried to UHP depth during continental subduction. Therefore, a simple idea that



FIG. 6. – Fluids, as shown by the numerical models [after Faccenda *et al.*, 2009] should play a major role in localized yielding of the lithosphere at the subduction sites. They also are responsible for the asymmetry of subduction. Fluids penetrate in normal faults initialized by flexural deformation (fig. 5) resulting both in pressure drop and serpentinization, hence, additional weakening of the plate at the inflexion point as well as in weakening of mantle-crustal interface. Flexurally induced normal faulting can also explain seismic anisotropy characterizing the subduction interface.

continental subduction can be made possible by skinning-off its low density upper crust is probably not universally valid. The driving mechanisms and plate-interface weakening processes that enable continental subduction are still not clear but the presence of thick, relatively weak and rheologically stratified crust as well as localized mechanical softening and density changes due to metamorphic transformations appear to play an important role [e.g., Burov et al., 2001; Yamato et al., 2008]. Preservation of slab integrity is a major problem for continental subduction, since continental convergence occurs at much slower rates than in oceans. Oceanic subduction typically takes place at rates of 5-15 cm.yr⁻¹, which implies relatively high (> 10)Peclet numbers (Peclet number is the ratio of the rate of heat advection to that of heat conduction). This practically means that cold oceanic slabs subduct so rapidly that they have no time to heat up (and hence reduce their strength) due to conductive heat exchanges with the surrounding asthenosphere before they reach significant depths (if the subduction dip is steep enough). As a consequence, steep-dip oceanic slabs break-off only by the moment when they have already sunk to great depths. In continents, convergence rates are much slower, sometimes not exceeding several mm.yr⁻¹. Under these conditions, the lithosphere may heat up, thermally weaken and break-off well before it reaches HP depths. It is therefore evident that the conditions for continental subduction cannot be assessed in a simple way and require a numerical modelling approach combining all of the key factors affecting the convergent

processes. All of the above mentioned factors could not be treated within simple conceptual or analytical considerations, analog or conventional numerical models, and required major development of the numerical modelling techniques. For these reasons, thermo-mechanical models of continental subduction and exhumation are very recent (the first model of this kind was published in 2001 by Burov *et al.*). Since 2001 this domain has been addressed by a growing number of numerical studies (fig. 10) [Yamato *et al.*, 2008; 2009; Gray and Pysklywec, 2012; Francois *et al.*, 2013; Sizova *et al.*, 2013] that demonstrated physical possibility of continental subduction – until recent doubted by many geologists – in various settings and helped defining the particular mechanisms behind this enigmatic process.

The new generation of observation-oriented models that have allowed for this major progress have among particular features the capacity of treating new multidisciplinary types of data and processes such as the data of metamorphic petrology and phase changes or denudation data and surface processes. For example, if one considers P-T conditions inferred for subduction zones, then UHP material should have been buried to depths of 100-150 km and brought back to the surface. The corresponding P-T and P-T-t paths not only demonstrate this possibility but also provide quantitative constraints, via P-T and P-T-t trends of the particular dynamics of the subduction (burial) and exhumation processes. Provided that the UHP depth estimates are correct



FIG. 7. – Fluids should also play a major role in exhumation of the metamorphic facies and lubrication of the subduction channel [Angiboust *et al.*, 2012]. The models show strong impact of fluids and metamorphic reactions on the dynamics on the subduction zone dynamics.

[e.g., Spear, 1993], the HP/UHP rocks can be regarded as direct markers of continental subduction and their P-T-t paths can be used for reconstruction of subduction dynamics and of the conditions at the subduction interface. Under these assumptions, detailed studies of HP/UHP rocks provide new direct constraints on thermo-mechanical processes in subduction zones [Coleman, 1971; Ernst, 1973; 2010]. These data can provide insights on the mechanisms of exhumation as well, since different processes and contexts would potentially result in different styles of deformation and hence in different P-T-t paths. In particular, based on the analysis of metamorphic data [Ernst, 2010], it has been suggested that two main types of continental convergence can be distinguished: fast "Pacific underflow", where continental subduction is preceded by that of thousands of kilometres of oceanic lithosphere, and slow "Alpine closure" of an intervening oceanic basin leading to short-lived continental subduction (simple shear) soon followed by lock-up of the subduction channel leading to switching to pure shear deformation mode (fig. 3). It has been also pointed out that the exhumed HP-UHP complexes display low-aggregate bulk densities [e.g., Ernst, 2010], while the exhumation rates in some cases largely exceed the convergence rates [e.g., Yamato et al., 2008] (fig. 11), jointly suggesting a buoyancy-driven (Stokes flow) ascent mechanism, the idea that has been successfully tested in Burov et al. [2001] and Yamato et al. [2008]. By now, a large number of modelling studies have investigated various factors influencing subduction processes [e.g., Doin and Henry, 2001; Pysklywec et al., 2000; Sobouti and Arkani-Hamed, 2002; Chemenda et al., 1995; Gerya et al., 2002; Yamato et al., 2007, 2008; Warren et al., 2008a,b; Sizova et al., 2010; Gray and Pysklywec, 2010; 2012]. However, not all of the existing models fully match for the task. As mentioned, the analogue models are largely inadequate because of impossibility to incorporate phase changes, rheological simplifications and fairly scaled thermal coupling. The numerical models are often limited by simplified visco-plastic rheologies or by the rigid top/"sticky air" upper-boundary condition, often implemented in Eulerean codes instead of free-surface boundary condition. The use of rigid-top upper-boundary condition forces stable subduction [Doin and Henry, 2001; Sobouti and Arkani-Hamed, 2002], attenuates pure shear, cancels folding and does not allow for consistent prediction of topography evolution. Many models also do not incorporate surface processes, which are key forcing factors of continental collision [e.g., Avouac and Burov, 1996] and an integral part of the final stages of exhumation

[e.g., Yamato *et al.*, 2008]. Some studies also force a specific convergence mode, in particular, subduction, via prescription of favoring boundary conditions, for example, by putting an additional boundary condition (e.g., "S-point") inside the model [e.g., Beaumont *et al.*, 1996; Beaumont *et al.*, 2000]. Some models are also inadequate because they favor pure shear collision by including a weak zone in the plate shortened in the direction opposite to the pre-imposed mantle flow [Pysklywec *et al.*, 2002]. Finally, models operating in deviatoric stress formulation may also face specific difficulties with evaluation of total pressure needed correct account for brittle deformation and P-T-t conditions. Even though some earlier modelling studies [Burov *et al.*, 2001; Toussaint *et al.*, 2004a,b; Burg and Gerya, 2005; Gerya *et*

al., 2002] included simplified phase change algorithms,

fully coupled models with progressive phase changes directly derived from thermodynamic relations have emerged only few years ago [Stöckhert and Gerya, 2005; Yamato *et al.*, 2007; Li and Gerya, 2009; Li *et al.*, 2010; 2011; Burov *et al.*, 2012; Francois *et al.*, 2013].

Summarizing the requirements to the numerical models of collision and exhumation, we can conclude that they should: (1) allow for all modes of deformation, (2) account for viscous-elastic-plastic rheology and thermal evolution, (3) be thermodynamically coupled, i.e. account for phase changes (and at best for fluid circulation), (4) account for surface processes and free-surface boundary condition (or at least incorporate "sticky air" approximation of the free surface), (5) provide an accurate solution for total pressure.



FIG. 8. – Examples of 2D numerical models of subduction resulting in spontaneous oceanic slab break-off during continental collision [Duretz *et al.*, 2011, see also Gerya, 2011]. (a) Four stages (top diagrams) of model evolution for the shallow slab break-off regime and associated surface topography development (bottom diagram). During slab necking and break-off, the subducted crust deforms in a brittle manner and the mantle lithosphere deforms viscously. (b) Four stages (top diagrams) of model evolution for the deep slab break-off regime and associated surface topography development (bottom diagram). During slab necking and break-off, the subducted crust deforms viscously and the mantle lithosphere deforms both viscously and by Peierls mechanism.

It is hence evident that a joint modelling approach considering collision processes in direct relation to exhumation, fluid circulation and formation of HP/UHP material is needed for understanding both the mechanisms of continental convergence and of UHP/HP exhumation.

By reproducing more and more sensible observations, the models allow us to understand the complexity and conditions of various factors involved in the oceanic and continental convergence. Due to the involvement of so many different factors, it is generally impossible to reduce these processes to simplified sketchy concepts

RIFTS AND MARGINS

Lithospheric extension is associated with tectonic deformation and/or magmatism governing formation of rifts and conjugate



FIG. 9. – Example of 3D oceanic subduction [Burkett and Billen, 2010; van Hunen and Allen, 2011, see also Gerya, 2011]. 3D numerical models show the possibility of slab break-off due to ridge–trench collision (a, b) [Burkett and Billen, 2010] and continental collision (c, d) [van Hunen and Allen, 2011]. (a, c) Detachment of laterally symmetric slabs. (b, d) Detachment of laterally asymmetric slabs: (b) slab with two offset ridge segments separated by weak fracture zone, (d) only part of the slab has a continental block. Slab width is 300 km in (a, b) and 2,000 km in (c, d). The 1050°C isosurface is shown in (a, b) and 945°C in (c, d).

margins. Continental rifting begins with extensional stress applied to the lithosphere, laterally or from below, until it thins and eventually breaks apart, culminating in crustal rupture and creation of a new oceanic lithosphere accommodating the plates separation [see review by Ziegler and Cloetingh, 2004].

Due to their key role in geodynamics and their specific importance for mineral exploration, rifted basins and margins have been extensively studied by various observational methods as well as by analogue and numerical modelling. At the beginning, a very important contribution to understanding of syn-rift processes and of the importance of rheological stratification of the lithosphere has been made by analogue modelling [e.g., Brun, 1999]. In particular, the analogue modelling studies have shown that rift structure and rifting styles are largely controlled by the rheological properties and relative integrated strengths of crustal and mantle layers. The analogue models have also demonstrated that ductile flow in the lower crust should strongly affect rift evolution and, contra-intuitively, control localization and distribution of faults and tilted blocks at the surface [Brun, 1999]. Post-rift subsidence stages are, however, strongly affected by thermo-mechanical interactions as the large part of the post-rift subsidence is controlled by thermal cooling leading to density increase [McKenzie, 1978] and progressive mechanical strengthening of initially weakened lithosphere [Burov and Poliakov, 2001]. The numerical models have shown here that pure thermal subsidence due to cooling [McKenzie, 1978] is insufficient to explain post-rift evolution of rifted lithosphere since ductile strength recovery, gravitational instabilities and phase changes may largely interfere at this stage. For example, it has been demonstrated that at some stage, thinned lithosphere becomes stronger that it was before the rifting episode [Burov and Poliakov, 2001], which results in increasing flexural resistance and hence in eventually strong decrease of the amplitude of thermal subsidence (compared to McKenzie model). Since post-rift evolution of sedimentary basins is of particular interest for industrial exploration, the thermo-mechanical numerical models of post-rift subsidence have progressively taken an essential part in basin studies.

First models of formation of rifts and rifted margins predicted uniform thinning of the continental crust accommodated by tilted blocks that, in case of margins, are juxtaposed to the oceanic crust along a sharp boundary. Two end-member conceptual models have first been proposed for describing how the continental lithosphere deforms and extends: (1) the pure-shear model [McKenzie, 1978] where the same amount of extension occurs in the upper and lower crust, generally producing symmetric rifted margins; and (2) the simple-shear model [Lister et al., 1986; Lister and Davis, 1989; Wernicke, 1985] where a low-angle shear zone extends through the entire lithosphere producing differential thinning of the crust and mantle lithosphere, and forming asymmetric rifts and margins. Combinations of these end-member mechanisms produce different styles of rift structures [e.g. Lister and Davis, 1989; Buck, 1991; Kusznir et al., 1991; Bassi et al., 1993]. Then, it has been shown that lithosphere necking can proceed to the break-up phase with or without lower crustal flow, affecting crustal thinning profiles [Braun and Beaumont, 1989; Hopper and Buck, 1996].

Thermo-mechanical modelling has been widely used not only to study the mechanisms of lithosphere extension but also for better constraining of the parameters governing the morphology of rifted structures [e.g. Dunbar and Sawyer, 1988; Bassi *et al.*, 1993; Burov and Cloetingh, 1997; Chéry *et al.*, 1989; Huismans *et al.*, 2001; Lavier *et al.*, 2000; Burov and Poliakov, 2001; Huismans and Beaumont, 2011; Tirel *et al.*, 2008; 2013; Watremez *et al.*, 2013].

Dynamic thermo-mechanical models have demonstrated their advantages (compared to analog models) not only for the analysis of the impact of thermal conditions but also for that of boundary conditions, such as extension velocity and surface erosion (fig. 12 and 13). In difference from most analog models, the numerical models have demonstrated that extension velocity is a key parameter governing the focusing of deformation and lithosphere breakup (fig. 14); [Huismans *et al.*, 2005]. In addition, they have shown that there, important implications of the lithosphere rheology with respect to extension, in particular, the relationship of viscous flow power-law exponent and development of necking [Fletcher, 1974; Schmalholz *et al.*, 2008] and Moho geometry [e.g., Tirel *et al.*, 2008]. The influence of melting-related weakening and other strain localization processes such as



FIG. 10. – Example of continental subduction models [Francois *et al.*, 2013] showing initiation of a continental slab detachment some time past the oceanic slab break-off.

(kbar)

30

10

formulation FIG. 11. – Example of continental subduction models [Yamato *et al.*, 2008] applied to slow Alpine collision. The model uses P-T-t data for better constraining of the subduction zone dynamics, and for explanation of UHP exhumation to the surfcae. The right part of the figure shows the match between the observed UHP data and the predicted P-T paths.

950

20 Myr

X (km)

850

thermally and themo-dynamically coupled

inherited tectonic heterogeneities [e.g., Le Pourhiet *et al.*, 2004] have been also shown to be considerable. For instance, Huismans and Beaumont [2003; 2007] and Huismans *et al.* [2005] have demonstrated that localization of deformation and rift mode selection during extension may be closely related to dynamic weakening; some recent publications emphasize several physical mechanisms to explain this weakening such as shear heating [Kaus and Podladchikov, 2006; Crameri and Kaus, 2010], damage evolution [Karrech *et al.*, 2011], grain size reduction [Braun *et al.*, 1999], lattice preferred orientation [Tomassi *et al.*, 2009] and some other mechanisms such as fluid-induced metamorphic reactions at different crustal levels [Mohn *et al.*, 2011].

Understanding the mechanisms of formation of the continental margins presents a particular challenge for geodynamic models. Application of the numerical models to the data of field observations has already provided an improved knowledge of the process leading to the formation of rifted margins [e.g. Brun and Beslier, 1996; Lavier and Manatschal, 2006; Huismans and Beaumont, 2011]. One can mention here the important contribution of the numerical models to understanding of the dependence of the rifting style and margin morphology on the extension rate. This dependence has been first established from direct observations of the morphology of oceanic spreading centres where slow spreading centres (e.g. Antlantic ridge) exhibit strong structural differences (localized rifting) from the fast spreading

400

Predicted exumation P-T-t-z paths comparable

with petrology data

150'0



FIG. 12. – Extensional models: general conceptual setup. State of the art models account for elastic-brittle-ductile rheological structure of the lithosphere and surface processes (erosion and sedimentation).

O

100

0

100

200 -16

650

UCDP

Strain rate

LCDP

Deph (km)

centres (Pacific ridge, distributed rifting). However, the dependence of rifting style on the extension rate, well established for the oceans, has been long ignored for continental rifting and breakup (preceding formation of the continental margins). Salvenson's [1978] classification of rift morphology as a single function of the amount of crustal thinning (characterized by stretching factor β) has dominated for a prolonged period of time, until the thermally-coupled numerical models [Huismans and Beaumont, 2007; Burov, 2007] have shown that rifting styles and evolution of margins must be as strongly dependent on the extension rate as the oceanic rifts. It has been shown, for example, that slow extension (fig. 15) promotes development of strong gravitational instabilities that result in highly asymmetric rifting style, while fast extension promotes rift symmetry. Similarly, in difference from R. Buck [1991] hypothesis on predominate importance of the initial thermo-rheological profile on rifting style, it has been later demonstrated [Huismans and Beaumont, 2007] that the extension rate and mechanical softening may induce style variations comparable of the same order as the effect of the initial rheological stratification.

Based on thermo-mechanically-coupled numerical experiments, Burov [2007] suggested that slow extension may be associated with the development of gravitational instabilities in the lower lithospheric mantle along the margins of the area of mantle lithosphere thinning, resulting in its

sinking into the asthenosphere, and, hence, in strong additional "gravitational" thinning of the lithosphere by mantle lithosphere delamination (fig. 15). These instabilities develop because the mantle lithosphere is colder and thus denser than the hot asthenosphere (1330°C), which upwells to replace it in the zones of mantle lithosphere thinning, so that at each moment the degree of assimilation of the mantle lithosphere by the asthenosphere and the density contrast with them is limited by the ratio of thermal advection rate to thermal diffusion rate (Peclet number). If the extension rate is low enough, the characteristic time scale of growth of basal mantle-lithosphere gravitational instabilities becomes comparable or even smaller than the characteristic time scale of the syn-rift phase. These instabilities may eventually grow even at higher rates than the rate of lithospheric thinning by pure or simple shear.

Hence, the Rayleigh-Taylor instabilities interplay with rifting processes, potentially resulting in asymmetric rifting and/or in increased amount of thinning, specifically in the mantle part of the lithosphere. Mantle lithosphere delamination may also eventually lead to additional partial melting resulting from the ascent of the asthenospheric material to sub-moho depths (< 50 km). It can be further suggested that such delamination-caused partial melting can be generated even under non-volcanic margins. One of the other consequences of the mantle lithosphere instabilities



FIG. 13a. – Example of numerical experiments on extension [Burov and Polyakov, 2001]: reproducing basin morphology as function of the amount of crustal thickening (coefficient of extension β). The left part shows observationally constrained rift structures as function of β [Salvenson, 1978].



Frictional Plastic Strain Softening $\Phi(\epsilon) = 7 ---> 1 \ \epsilon = 0.5 ---> 1.5$

FIG. 13b. - Example of numerical simulation of rift basin formation in slow extensional context, assuming strong strain-softening of the material [Huismans and Beaumont, 2007].



Controls on asymmetry

FIG. 14. - Dependence of rifting style on the extension rate [after Huismans and Beaumont, 2007]. Thermomechanical models have demonstrated that rifting style and morphology largely depends on the rheological structure and extension rate, and not only on the stretching factor β the amount of extensional thinning). "Coupled / Decoupled" means, respectively, rheological coupling and decoupling between crust and mantle.

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predicted by the numerical experiments is the development of series of periodic changes in subsidence associated with delamination of dense mantle. To characterize the relative role of the gravitational instabilities during rifting, Burov [2007] introduced a special parameter, the "rift Deborah number":

$De_r = 13.04 \ \mu_{\text{eff}} \ u_x \ / \ (\Delta \rho g d \ L)$

where μ_{eff} is effective viscosity. Assuming a ductile flow law:

 $De_r = 13.04 \ \mu_0 \ exp(H/nRT) \ u_x \ / \ ((\Delta \rho_c + \alpha \Delta \rho_0 \Delta T)gd \ L)$

with $\mu_0 = e^{d_{\text{II}} (1-n)/n} (\text{A}^*)^{-1/n}$, $e^{d_{\text{II}}} = (\text{Inv}_{\text{II}} (e_{ij}))^{1/2}$ is the effective strain-rate and $\text{A}^* = 1/2\text{A}\cdot3^{(n+1)/2}$ is the material constant, H is the activation enthalpy, R is the gas constant, n is the power law exponent. L is the final width of the rift and u_x is the extension rate, $\Delta \rho_c + \alpha \rho_0 \Delta T = \Delta \rho$, $\Delta \rho_c$ is the compositional density contrast, α is the coefficient of thermal expansion, ρ_0 is the density at reference temperature and ΔT is the temperature change in respect to the reference temperature. Based on the results of modelling and analytical analysis, Burov [2007] has shown that gravitational instabilities play an important role for $De_r < 10$, specifically for $De_r < 1.5$. It is also noteworthy that Moho depth and geometry are largely controlled by extension and the evolution of mantle-lithospheric gravitational instabilities. In particular, slow extension may result in subsidence of the Moho during the syn-rift phase. Figure 15b shows the experiment where extension occurs at extension rate (10 mm/yr) corresponding to subcritical value of $De_r (De_r \sim 1)$ below which, inclusively, rifting can be treated as "slow" in terms of the impact of gravitational instabilities, so that Moho boundary remains almost flat or goes down instead of rising up. This experiment shows that, contrary to common assumptions, in case of deep lithospheric necking level, under low extension rates, the Moho may remain stable or even subside in response to lower mantle-lithosphere gravitational instabilities. Upon detachment of significant volumes of lithospheric mantle, the lithosphere may rebound and the graben flanks can be uplifted, even in the absence of further extension. The mantle detachment may occur in pace with thermal re-equilibration of the lithosphere so that the density contrast between the latter and the underlying mantle can be quite small at the moment when the detachment finally takes place. The models also show that the detachment may laterally migrate in the direction of the extension at rates exceeding extension rate. Hence, for relatively high extension rates, partial mantle delamination may occur at some distance from the rift flanks resulting in uplift of rift borders.

Rifted margins present another important challenge for the contemporary numerical models [e.g., Huismans and Beaumont, 2011] as their formation is associated with extreme deformation and intensive mantle-lithosphere interactions, after the lithosphere has been thinned by a factor higher than 5 [Salvenson, 1978]. Numerical models have been successfully used to address the most pertinent questions concerning evolution of rifted margin even though a number of questions such as impact of magmatic processes or formation of hyper-extended crusts still remains an open question.

Passive margins are usually separated into two large classes: volcanic or non-volcanic margins depending on whether magmatism have occurred during rifting or on later stages. Even if this classification is contested in terms of both the underlying mechanisms and observations [Huismans and Beaumont, 2011; Geoffroy, 2005], it still can be retained in terms of morphological structures. Non-volcanic rifted margins usually show tectonized features (tilted blocks) and a transitional zone between the continental crust and the oceanic crust called Ocean-Continent transition (OCT) [e.g. Lavier and Manatschal, 2006]. The nature of the OCT is fairly known and seems to vary from one non-volcanic margin to the other. This OCT usually exhibits (1) a zone of exhumed continental mantle (ZECM) [e.g. Manatschal, 2004]; or (2) a deeper mantle serpentinized by percolation of the seawater into the sediments and the faulted crust; or (3) a highly tectonized oceanic crust formed by ultra-slow spreading. Non-volcanic margins can



FIG. 15a. – Example of formation of a slow continental margin [Burov, 2007]: a conceptual model. The thermo-mechanical experiments suggest that slow rifting may be strongly influenced by competition between the advective and diffusive processes. If heat diffusion has same or faster characteristic time scales as heat advection, then gravitation instabilities develop, leading to gravitational removal of a large amount of mantle lithosphere, with strong consequences for surface evolution (e.g. enhanced thinning, uplift) and rift morphology.



FIG. 15b. – Example of a numerical study reproducing formation of a slow margin [Burov, 2007]: a numerical experiment exploring gravitational instability of the mantle lithosphere during extension. Left panel: blue color corresponds to the mantle lithosphere, yellow – to the lower crust, orange – to the upper crust, purple is the new oceanic crust and sediment, green is the asthenosphere (Colours refer to the PDF version).

also show a limited magmatism attributed to decompressional melting during crustal thinning or post-rift thermal anomaly. Volcanic rifted margins are characterized by large amounts of magmatism (basalt flows, volcanoes, mafic underplating) produced during the rifting process [e.g. Geoffroy, 2006], and an ocean-continent boundary or a very narrow OCT. Volcanic margins are commonly associated with high thermal anomalies in the mantle, allowing for formation of significant amounts of melt under extension [e.g. White and McKenzie, 1989]. Most of the above problems present a challenge for next generations of numerical models. In particular, the interplay between extension and magmatism during continental breakup is still debated and recent numerical modelling studies suggest that the volumes of melts extruded at volcanic margins may also be generated by 'standard' thermal conditions, provided high extension rates can be implied [Huismans and Beaumont, 2011]. The numerical models under development would necessarily need an account for melting and other fluid-rock interactions during the extensional processes, through development of bi-phase flow approach addressing hydration-dehydration reactions and porous flow in the extended crust [Mezri et al., 2013]. Since rock porosity appears to be pressure, temperature and strain-rate dependent [Angiboust et al., 2012 and references therein] while metamorphic reactions also require presence of fluids, which have also strong impact on the brittle and ductile rock strength, one can suggest that there may be a strong coupling between tectonic and fluid circulation mechanisms in the extensional context.

Many fundamental questions remain unsolved and require further modelling efforts concerning the evolution of volcanic and non-volcanic margins. In particular, it is still not clear how the properties of the mantle lithosphere – except its thermal state and ductile strength – affect rift evolution. For example, the idea that common plastic failure criterion [Byerlee/Mohr-Coulomb, Byerlee, 1978] may not be applicable to the mantle lithosphere has been widely discussed in the recent literature [e.g. Burov, 2011; Precigout *et al.*, 2007; Watts and Burov, 2003]. It is suggested that this criterion may largely overestimate the mechanical strength of the lithosphere [e.g., Precigout *et al.*, 2007], leading to incorrect prediction of such key features as timing of continental break-up and margin geometry.

INTERPLAY BETWEEN LITHOSPHERE DYNAMICS AND SURFACE PROCESSES

Surface processes may play a significant role during both in subduction/collision processes [e.g., Dahlen and Suppe, 1988; Avouac and Burov, 1996; Beaumont et al., 2000; Pysklywec, 2006; Burov, 2010] syn-rift and post-rift evolution [e.g., Burov and Cloetingh, 1997; Burov and Poliakov, 2001], not only in terms of the effect of sediments on thermal blanketing causing temperature rise in sedimentary basins [e.g., Lavier and Steckler, 1997], or due to their lubricating effect on the subduction channel, but first of all due to the straightforward effect of lateral distribution of important surface loads carried out by erosion and sedimentation processes (fig. 16). In zones of fast tectonic deformation (i.e., horizontal convergence/extension rates $> \sim 1$ cm/y), surface processes modify topography at rates comparable with the rates of the tectonic uplift/subsidence (a few 0.1 mm/yr), leading, in some cases, to erosion of thousands meters of topography from mountains or from rift flanks and deposition of the equivalent amounts of sedimentary infill [e.g., Avouac and Burov, 1996; Burov and Cloetingh, 1997]. The associated dynamic loading and unloading exerted on the supporting crust and lithosphere is on the same order as tectonic loading, suggesting possible strong feedbacks between the surface and tectonic processes. In particular, an increase of sedimentary loading may lead to localised yielding and deflection of the supporting lithosphere. At the same time, erosional unloading of orogenic belts or on rift shoulders leads to their flexural or isostatic uplift and strengthening. Of specific importance, according to some models, is also the "localizing" effect of erosion on faulting [e.g., Burov and Poliakov, 2001]. Surface processes, potentially resulting in acceleration of orogenic processes in collisional contexts or in enhanced subsidence and extension of rifted basins and uplift of the rift shoulders, create pressure gradients sufficient to drive ductile flow in the low-viscosity lower crust (fig. 16) [Burov and Cloetingh, 1997]. It must be noted, however, that the feedbacks between tectonics and surface process are most important in regions characterized by high rates of tectonic uplift or subsidence (such as India-Asia collision). Numerical models have shown that in slowly evolving regions such



FIG. 16. – Interplay between surface and subsurface processes: concept illustrating possible feedbacks between surface processes and subsurface response through ductile flow in the crust and mechanical response of the lithosphere to loading/unloading.

as western Alpes, the "tectonic" impact of surface processes is rather insignificant [e.g., Yamato *et al.*, 2008].

The complex interplays between surface processes, climate and tectonic deformation can be only assessed through physically consistent thermo-mechanical modelling. Models have shown the importance of isostatic effects associated with variations in surface loading caused by surface processes. They have demonstrated as well that crustal ductile flow may indeed occur until the ductile channel thickness is greater than a few km [Burov and Cloetingh, 1997] thus allowing for dynamic feedback between surface loading and subsurface deformation. This flow is also largely gravity driven, due to lateral Moho gradients associated with crustal thinning. In case of rifting, for example, the flow rate first progressively increases as the crust thins, and then decreases when there is no more ductile crustal material below the rift zone. This flow, directed outward from the centre of the basin may facilitate uplift of the rift shoulders (figs 16-17) [Burov and Poliakov, 2001]. It may even drive some post-rift "extension" [Burov and Poliakov, 2001]. In the limiting case of slow erosion and sedimentation rates, gravitational stresses can reverse the flow, resulting in retardation of basin subsidence rate, homogenisation of the crustal thickness, accelerated collapse of the shoulders and in some post-rift "compression". These effects may significantly change predictions of basin evolution inferred from the conventional stretching models.

Similarly, models of continental collision have revealed a strong potential dependence of the collision style on the intensity of surface processes and the degree of their interaction with the subsurface deformation. It has been shown that [Burov and Toussaint, 2007] in case of fast convergence rates (> 3 cm/y), there should be a very strong coupling between surface and subsurface processes so that not only the topography growth rates but also deep processes such as the amount of subduction are strongly affected by surface erosion. In particular, it has been demonstrated that in "Himalayan context", coupling between surface and subsurface processes controls as much as 50% of the total amount of the subducted continental lithosphere [Toussaint *et al.*, 2004b]. It has been even proposed, based on ductile crustal flow models [Beaumont *et al.*, 2001], that the erosion is strong enough to drive the exhumation of the ductile crust of Tibet in the Himalayas, although these former ideas seemingly do not find sufficient confirmation from recent field observations [Searle *et al.*, 2011; Searle, 2013]. However, as mentioned, in case of slow convergence rate [Yamato *et al.*, 2008] the role of surface processes is far less significant.

MANTLE-LITHOSPHERE INTERACTIONS

Mantle convection and plumes are thought to constitute "engines" of plate tectonics. The problem of mantle-lithosphere interactions has been largely addressed by thermomechanical models due the principal difficulty to obtain any direct information about deep processes. The geophysical methods such as seismic tomography or gravity show only current, generally ambiguous snapshots of the Earth interiors while the interpretations of the impact of mantle dynamics on surface and tectonic deformation records are also subject of strong assumptions. Numerical models thus have played an essential role in the improvement of our understanding of the potential features of surface and tectonic response to mantle flow, in particular, dynamic topography and deformation fields produced by mantle plumes. Based on these models, it has been only recently shown that dynamic topography (i.e. surface undulations created by mantle upwellings and downwellings) may exhibit contre-intuitive features being strongly impacted by the rheological properties of the lithosphere. Burov and Guillou-Frottier [2005], for



FIG. 17. – Interplay between surface and subsurface processes: example of a viscous-elastic-ductile numerical model of extension of a young lithosphere [Burov and Poliakov, 2001]. The left panel: extension of the lithosphere in the absence of extension. Right panel: extension of the lithosphere in presence of syn-rift erosion with erosion coefficient k of 1000 m²/yr. For comparison, topography profile for $k = 500 \text{ m}^2/\text{yr}$ is also shown.

example, have shown that in contrast to usual expectation of long-wavelength surface deformation, the dynamic topography may in reality mainly present short-wavelength features (fig. 18). The resulting thermo-mechanical consequences for surface geodynamics and geology appear to be largely dependent not only on the characteristics on the mantle upwelling, but also on the thermo-rheological and density structure of the lithosphere [d'Acremont *et al.*, 2003; Burov



FIG. 18. – Dynamic topography over continents as revealed by thermo-mechanical models accounting for rheological stratification of the lithosphere [Burov and Cloetingh, 2010]: general concept. Left panel shows common intuitive assumption about dynamic topography in which the lithosphere is considered as a stagnant lid passively transmitting mantle motions to the surface. Right: a concept accounting for rheological stratification and free surface of the lithosphere suggesting that dynamic topography can be largely accommodated within the ductile crust, and overall modulated by crustal and lithosphere mantle deformation. In this case the long-wavelength will be attenuated and tensional/compressional instabilities in lithospheric layers may generate short wavelengths overprinting the long-wavelength signal.



FIG. 19. – Dynamic topography evolution predicted by a numerical model [Burov and Gerya, 2014], in which mantle plume interacts with stratified viscous-elastic-ductile lithosphere. The lower panel shows density anomaly field associated with plume-mantle-lithosphere interaction. The upper panel shows induced topography evolution.

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FIG. 20. – Example of a high-resolution 3D numerical model of evolution of crustal rifting patterns and plume geometry during plume-lithosphere interaction in presence of far-field tectonic stress (which direction in shown with grey arrows) applied to the lithosphere. The figure represents combined shear strain rate patterns (near surface horizontal sections) and material phase distribution [after Burov and Gerya, 2014; Burov *et al.*, 2014].

and Guillou-Frottier, 2005; Burov *et al.*, 2007; Burov and Cloetingh, 2009; 2010]. The models have demonstrated that both the thermo-tectonic age and rheological stratification of the lithosphere have a strong impact on the effect on mantle-lithosphere interactions [Burov and Guillou-Frottier, 2005]. As a result, the presence of low-viscosity ductile lower crust leads to essential damping of the long-wave-length dynamic topography and appearance of short-wave-length tectonic-scale features, associated with tensional and compressional instabilities in the crustal layers (figs 19 and 20). Certainly, the common assumption of a horizontally uniform lithosphere at the site of future lithosphere

break-up caused by uprising asthenosphere is probably not realistic, in a view of the abundant evidence from the geological record that incipient rifts and rifted margins are usually localized at suture zones separating stronger lithosphere. Examples include the Caledonides suture of Laurentia-Greenland and Baltica, localizing Late Carboniferous and Permo-Triassic rifting and subsequent continental break-up around 65 Ma in the Arctic-northern Atlantic and the rift systems created at the edges of the African cratonic lithosphere [Corti et al., 2004; Corti, 2005; Janssen et al., 1995]. It should be noted also some natural examples do not always fit these assumptions. For instance, the Labrador Sea opened orthogonally to the basement grain, whereas the North Sea rift cuts obliquely across the Caledonian basement grain [Ziegler, 1988]. Plume impingement may also occur at the onset of the post-rift phase or even later. In this case the rifted margin lithosphere has been thermally reset to very young thermo-mechanical ages for the thinned continental lithosphere and the adjacent oceanic lithosphere. Hence, further model developments, in 2D and 3D, are needed to take into account the impact of tectonic heritage and spatially variable plate structure on the consequences of mantle-lithosphere interactions.

CONCLUSIONS

Observation-driven hypothesis can be verified indirectly through eliminating those that prove to be incompatible with the predictions of physically and observationally consistent models. On the other hand, model-driven hypothesis can orient field and laboratory research towards the acquisition of new data that may either confirm or dismiss model predictions.

The numerical models allow us to evaluate the relative importance of different processes involved in geological evolution and serve as power tools for interpretation of the geological, geophysical, petrological and other observations. The numerical thermo-mechanical models play an essential role allowing one to understand the phenomena, which spatial and temporal scales go beyond the scale of human-scale observations. They play a particular role in validation [e.g., Burov *et al.*, 1999; Burov, 2011], or more precisely, refutation

TABLE Ia. - Summary of thermal and mechanical parameters used in model calculations [e.g., Turcotte and Schubert, 2002].

| Туре | Definition | Units | |
|------------|---|---|--|
| Thermal | Surface temperature (0 km depth) | 0°C | |
| | Temperature at the base of thermal lithosphere | 1330°C | |
| | Temperature at the base of upper mantle (650 km) | 1700° ±100°C | |
| | Thermal conductivity of crust | 2.5 Wm ⁻¹ °C ⁻¹ | |
| | Thermal conductivity of mantle | 3.5 Wm ⁻¹ °C ⁻¹ | |
| | Thermal diffusivity of mantle | $10^{-6} \text{ m}^2.\text{s}^{-1}$ | |
| | Radiogenic heat production at surface | $9.5 \times 10^{-10} \text{ W kg}^{-1}$ | |
| | Radiogenic heat production decay length | 10 km | |
| | Thermo-tectonic age of the lithosphere | 50 to 600 Myr | |
| Mechanical | Density of the upper crust [*] | 2700 kg m ⁻³ | |
| | Density of lower crust [*] | 2900 kg m ⁻³ | |
| | Density of oceanic crust* | 2900 kg m ⁻³ | |
| | Density of sediment [*] | 2600 kg m ⁻³ | |
| | Density of undepleted mantle [*] | 3330 kg m ⁻³ | |
| | Density of asthenosphere [*] | 3310 kg m ⁻³ | |
| | Lamé elastic constants λ , G (Here, $\lambda = G$) | 30 GPa | |
| | Byerlee's law – Friction angle | 30° | |
| | Byerlee's law – Cohesion | 20 MPa | |

* We here provide average densities, in thermo-dynamically coupled models densities are derived directly from the assumed mineralogical

composition as function of pressure and temperature conditions

TABLE Ib. – Example of ductile flow parameters assumed in model calculations. Compilation of Mackwell *et al.* [1998] based on data from Gleason and Tullis [1995], Hirth and Kohlstedt [1996], Chopra and Patterson [1981]. More recent data [see compilation in Bürgmann and Dresen, 2008] predict slightly different values for ductile flow parameters. However, on practice these differences are negated by adjusting geotherms or thicknesses of the rheological layers in a way that the integral strength of the lithosphere matches the observed T_e values.

| | | Pre-exponential | | |
|----------------------|---------------------------------|-----------------------------------|----------------------|-----------------------|
| | | stress constant | Power law | Activation energy, Q |
| Layer | Composition | А | exponent | KJ mol ⁻¹ |
| | | MPa ⁻ⁿ s ⁻¹ | n | |
| Upper Crust | Wet Quartzite | 1.1×10^{-4} | 4 | 223 |
| Lower | Dry Maryland Diabase | 8±4 | 4.7±0.6 | 485±30 |
| Crust | | | | |
| | Undried Pikwitonei granulite | 1.4×10^4 | 4.2 | 445 |
| Mantle or Oceanic | Dry Olivine | 4.85×10^4 | 3.5 | 535 |
| lithosphere | | | | |
| | Wet Olivine | 417 | 4.48 | 498 |
| | Diffusion creep | 1.92×10^{-4} | 1 | 3.0×10^2 |
| | Peierls law | 10 $^{7.8}$ ×10 $^{-12}$ | Peierls stress= 5GPa | 5.35 ×10 ² |

of geodynamic and geological hypotheses and for interpretation of various kinds of observations. The models serve also for validation, calibration and integration of different types of multidisciplinary data allowing one to elucidate the inconsistency in the data and validate extrapolations of these data to geological time and spatial scales. In particular, the data of rock-mechanics obtained at short and small laboratory scales can be tested through geodynamic models that can show at which extent the extrapolation of these data is valid. For example, seismic tomography images can be tested in terms of their compatibility with gravitational and mechanical stability of the mantle. The models serve also for directing field and laboratory research by showing sensibilities of studied processes to particular kinds of data thus suggesting which type of data needs to be acquired or sampled with improved accuracy.

The current challenges in the geodynamic modelling include further development of multi-process physically consistent models based on realistic viscous-plastic-rheologies. In particular, incorporation of thermodynamic processes such as phase changes and fluid percolation (porous flow) is on the neck of the art. Integration of surface processes is also an important challenge, especially in 3D, while expanding the geotectonic models down to the bottom of the upper mantle to take into account mantle lithosphere interactions is another paramount requirement. There is also a growing demand in terms of better spatial resolution of the models that should progressively reach that of field observations. In particular, tectonic scale models would ideally have spatial resolutions on the order of 100-1,000 m for grid resolutions on the order of 1,000-10,000 elements in single direction. Such resolution is a big algorithmic and methodological challenge in case of 3D models since it requires enormous computing resources and hence enormous code optimization efforts. Actually most advanced matrix inversion algorithms developed in the applied mathematics are limited to 1000³ implying that accessing higher resolutions would need strong cooperation between geodynamic modellers and specialists in applied mathematics.

It is finally important to remind that geotectonic models are naturally simpler than the objects (in other sciences such as engineering, computer models can be as complex as their targets). They are also based on potentially erroneous knowledge of model parameters since the geological and geophysical data used for their construction are "blurred" due to numerous uncertainties. This has to be retained while interpreting results of numerical modelling.

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