Computational Mechanics:

Bridging the Gap between Science and Technology

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Computational Mechanics is nowadays an indispensable scientific tool for developing new technologies and optimizing existing ones. In the Computational Mechanics field, the interaction between new scientific developments and technological applications is not only very fast but also very natural: industry continuously demands the capabilities for analyzing technological problems of increasing complexity and therefore the advances in computational methods are almost immediately applied for modeling technological applications.

Since technological decisions, with high influence on the ecological impact of industrial facilities, on labor conditions and on revenues, are reached based on the results provided by computational models, it is evident that these models have to be highly reliable. Therefore, it is of utmost importance that sound modeling techniques are used, that highly educated engineers develop the models and that the model outputs are subjected to experimental validation using either industrial or lab determinations.

In the development of computational models we can recognize four different steps:

❒ The identification of the physical phenomenon that is going to be analyzed and the isolation of its most relevant features.
❒ The formulation of the mathematical model, usually in the form of a PDE system with its proper domain definition, boundary and initial conditions, etc. Here we have to make important decisions on which aspects of the technological process physics are relevant and, therefore, need to be considered in the model, and which aspects are not; in this level we introduce hypotheses about the material response, friction, loads, etc. It is important that when an engineer analyzes the results provided by the mathematical model she/he checks the adequacy of those hypotheses.

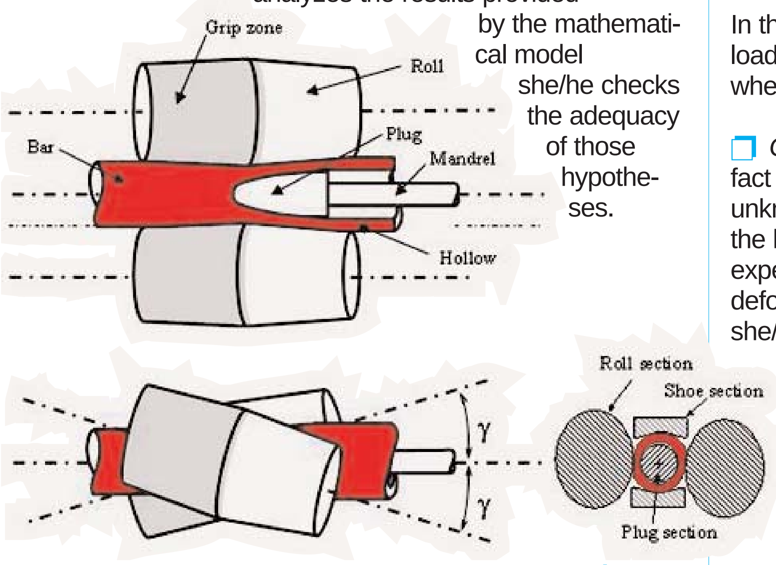


Figure 1:
The Mannesmann piercing process

❒ The formulation of a numerical model. In most cases the PDE system developed in the previous step cannot be solved in closed form; hence, it is necessary to get approximate solutions using numerical methods. In this paper we will focus on the finite element method.
❒ The verification of the numerical results where we check that they are a *"good enough"* solution for the mathematical model and the validation of the complete procedure where we check that the numerical results represent *"closely enough"* the physical phenomena under study.

The examples that we use to illustrate this paper are taken from actual applications that we developed for the steel industry.

From the physical phenomena to the mathematical model

Here the keyword is *abstraction*: the analyst should have enough insight into the physical phenomena that she/he has to model so as to include in the model all the relevant features but only the relevant ones. The educated physical intuition of the analyst together with a clear definition of the expected outputs is fundamental for the definition of an adequate mathematical model.

Due to geometrical or material nonlinearities most of the models that describe physical phenomena of technological relevance are nonlinear.

In the analysis of a solid under mechanical and thermal loads some of the nonlinearities that we may encounter when formulating the mathematical model are [1]:

❒ *Geometrical nonlinearities:* they are introduced by the fact that the equilibrium equations have to be satisfied in the unknown deformed configuration of the solid rather than in the known unloaded configuration. When the analyst expects that for her/his purposes the difference between the deformed and unloaded configurations can be neglected she/he may disregard this source of nonlinearity obtaining an important simplification in the mathematical model. An intermediate step would be to consider the equilibrium in the deformed configuration but to assume that the strains are very small (infinitesimal strains assumption). This also produces an important simplification in the mathematical model. Of course, all the simplifications introduced in the mathematical model have to be checked for their properness when examining the numerical results

- *Contact-type boundary conditions:* these are unilateral constraints in which the contact loads are distributed over an area that is a priori unknown to the analyst.
- *Material nonlinearities:* elasto-plastic material models (e.g. metals), creep behavior of metals in high-temperature environments, nonlinear elastic materials (e.g. polymers), fracturing materials (e.g. concrete), phase changes in solid state, etc.

In the analysis of a fluid flow under mechanical and thermal loads some of the nonlinearities that we may encounter when formulating the mathematical model are:

- *Non-constant viscosity / compressibility:* rheological materials and turbulent flows modeled using turbulence models.
- *Convective acceleration terms:* for flows with Re>0 when the mathematical model is developed using an Eulerian formulation, which is the standard case.

In the analysis of a heat transfer process some of the nonlinearities that we may encounter when formulating the mathematical model are:

- *Temperature dependent thermal properties:* e.g. phase changes.
- *Radiation boundary conditions.*

The numerical model

When using the finite element method for developing the numerical model, the first step is the selection of an adequate element formulation to be used in the discretization of the mathematical problem under consideration.

The finite element formulation has to fulfill the standard reliability criteria [2-4]:

- Fulfillment of Irons' Patch Test.
- The element formulation must not contain spurious zero energy modes, must be stable and must not lock [5].
- The element predictions must be robust and quite insensitive to element distortions. For 2D four-node elements, used in solid mechanic applications, MacNeal [6] showed that a complete insensitivity to element distortions is incompatible with the fulfillment of the Patch Test; hence, in this case we have to give up some insensitivity to element distortions since we cannot wave Irons' test.

In particular, for solid mechanic models:

- When we expect a plastic strain localization to be developed we have to use elements that can predict this behavior without unrealistic diffusion of the plastic deformation zone [7]
- In those cases in which we expect a brittle-type of failure localization, it is necessary to use elements enriched with a localization mode. In our papers [8-9] we developed a mesh-independent formulation for modeling these problems which does not require the use of a non-physical softening stress - strain relation.

Also, it is worth noticing, that there are a number of practical decisions that the analyst who builds the numerical model has to make regarding iteration techniques, iteration tolerances, time-integration methods, direct or iterative solvers that may require special preconditioners [10], parallelization techniques, etc.

The numerical model inputs

Once the numerical model has been conceptually established it is necessary to input its data.

For elaborating the geometrical data, the development of finite element models from CAD files is a field in continuous expansion [11].

Regarding the material data, once we decide on the constitutive model to use, we need to resort to an inverse analysis methodology to determine the required material constants from experimental results. In previous publications we have analyzed some actual applications in the steel industry where we used inverse analysis procedures for determining material parameters from high temperature torsion tests and heat transfer coefficients from the indication of thermocouples installed in the mold of a continuous casting facility [12-15].

The verification of the numerical models and of its software implementations

In the verification process we have to prove that we are solving the equations right, and therefore this is a mathematical step [16]. In this step we have to show that our numerical scheme is convergent and stable.

Our basic tools in this step are: Irons' Patch Test (impossible to wave it!!), examination of the element eigenvalues under different geometric configurations, mesh refinement studies under different geometric configurations, stability and locking analyses for different values of the material parameters within the range of interest for the application, etc. It is important to notice that the verification process is not only related to a numerical procedure but also to its actual implementation in software (either commercial software or an in-house one) [16].

The next step is the training of analysts in the use of the simulation code. If a code is intended for the use of other analysts apart from the code developer, it is necessary to provide: adequate documentation where the range of applicability and limitations of the code should be clearly specified; user manuals and a set of benchmark problems to be used for testing the code installation and the analysts' understanding of the users manual.

Figure 2:
The three analyzed cases

	Profile scheme	Bar diameter
Case 1		395 mm
Case 2		395 mm
Case 3		215 mm

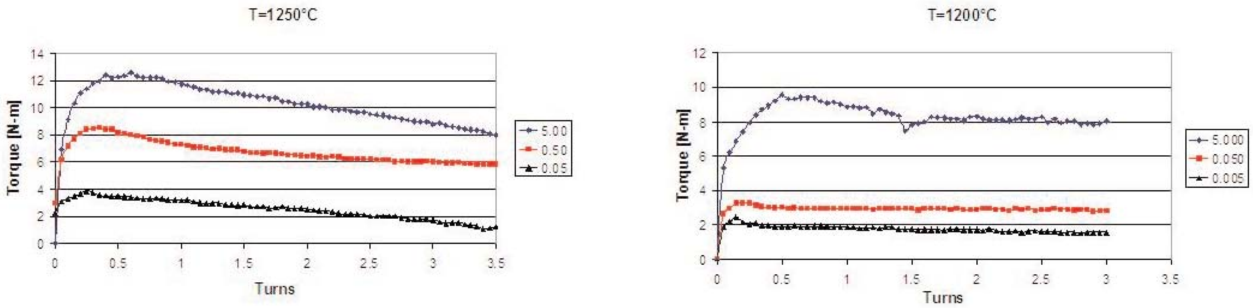


Figure 3:
Torque – turn curves for temperatures of 1200°C and 1250°C; with rotational speeds corresponding to 5; 0.5 and 0.05 turns/sec.

Figure 4:
Plug profile # 1. Comparison between the numerical results and experimental determinations.

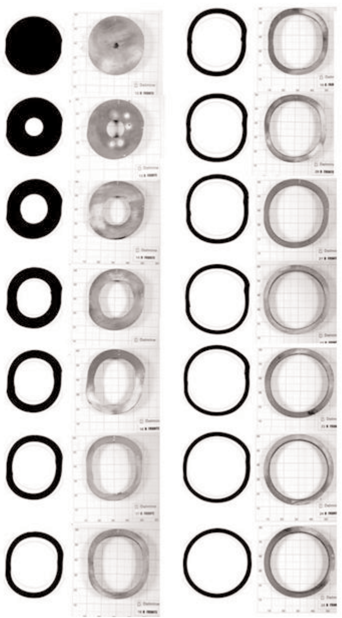


Figure 5:
Section through the rolls. The color map indicates the equivalent plastic strain and the dots the mapped data.

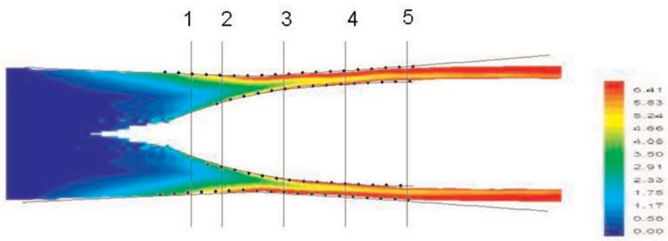
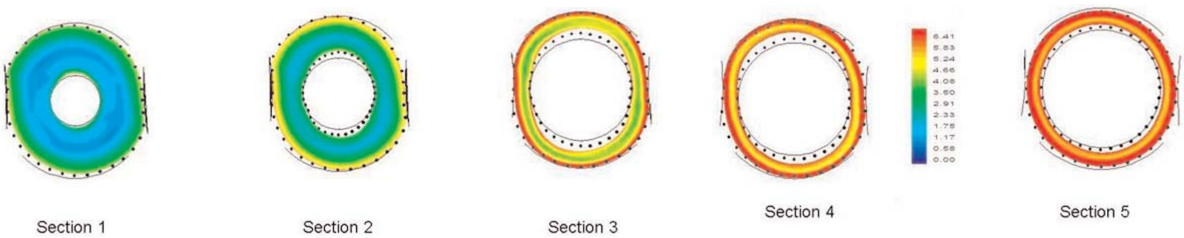


Figure 6:
Transversal sections (indicated in the previous figure). The color map indicates the equivalent plastic strain and the dots the mapped data.



The training of the analysts is particularly important in the case of commercial codes where it is necessary to confront the wrong concept that there is software that does not require from the users any insight into its mechanical and numerical bases.

The validation of the a computational model

In the validation process we have to prove that we are solving the right equations, and therefore it is an engineering step [16]. We do validate neither a formulation nor software: we validate the usage of verified software when used by a designed analyst in the simulation of a given process. We have to validate the complete procedure.

We can validate the computational model of a technological process by comparing the numerical results it provides with:

- Results obtained in the technical literature. This validation procedure serves only as a first approach, because usually the data that can be found in the literature is not complete enough to be used for a final model validation.
- Experimental results obtained in a laboratory. Of course, this is not a straightforward step because it has to be first proven that the laboratory set-up is an acceptable physical model of the technological process that we want to investigate. Hence, this is an involved two steps process: first we need to validate the physical model and afterwards use it to validate the numerical model.
- Results measured in the actual industrial process. This procedure provides the most reliable validation; however it is very expensive (an industrial facility has to be used during several hours as a lab) and difficult to control.

As illustrative examples of the last procedure, in the next sub-sections we are going to comment on the validation of computational models that we developed for a world class industry that manufactures seamless steel pipes.

Finite element model of the Mannesmann process

The Mannesmann process is used to produce hollow bars starting from circular cylindrical casted bars. To simulate this process, described in Fig. 1, we used a rigid/viscoplastic material model [17] implemented in our code METFOR using the pseudo-concentrations technique [18-19]. Details on the implementation and verification of the numerical technique are discussed in Refs. [20-24]. In Ref. [15] presented the model validation, that was performed by comparing the numerical results with industrial determinations.

The cases described in *Fig. 2* were analyzed in the validation process: the three cases correspond to the piercing of bars made with the same steel; the torque-turn curves of this steel were experimentally determined and a couple of them are shown in *Fig. 3*. By post-processing these experimental results we got the material parameters corresponding to an exponential-power law [12]. Isothermal analyses were performed considering a temperature of 1200°C.

A very sensitive parameter for comparing the numerical and industrial results is the pitch of the helix where the points initially on a straight line along the bar surface get located on the final hollow. This torsion helix is an important factor affecting the total redundant deformations that are introduced in the material by the piercing process. For cases 1 and 2, in *Table I* we compare the numerical and industrial results. In both cases the piercing process was interrupted with the blank inside the machine.

Plug	Elements	dof	FEM Pitch	Exp. Pitch
1	96,576	314,097	1158mm	1054mm
2	100,950	327,444	714mm	695mm

Table I:
Comparison between numerical and experimental results

In *Fig. 4* we compare, for the plug profile # 1, the first fourteen transversal cross sections determined with the model and the corresponding cross sections obtained during the industrial experiment.

In the third case the piercing process was also interrupted with the blank inside the machine. The outer surface of the semi-processed bar was mapped using the *"shapemeter"* described in Ref. [25]; the inner surface shape was replicated using a resin cast and the shape of the replica was also mapped as described in the cited reference. In *Figs. 5 & 6* we present, for this case, the comparison between the finite elements determined and experimentally mapped surfaces.

Model stability

In the development of the model several assumptions were made regarding the values of the friction coefficients and the length of the Mannesmann fracture cone [15]; hence, we have to investigate the stability of the results when those assumed physical parameters change. In Table II we summarize the numerical results.

Plug	μ_{rolls}	μ_{shoes}	μ_{plug}	$L_{Mann.}$	FEM-pitch	$\frac{FEM\ pitch}{Exp.\ pitch}$
1	0.2	0.2	0.35	150 *mm*	1054 *mm*	0.88
1	0.5	0.2	0.35	150 *mm*	1252 *mm*	1.05
1	0.2	0.2	0.35	300 *mm*	1158 *mm*	0.97
2	0.2	0.2	0.35	150 *mm*	695 *mm*	0.88
2	0.5	0.2	0.35	150 *mm*	899 *mm*	1.14
2	0.2	0.2	0.35	300 *mm*	714 *mm*	0.90

Table II:
Stability analysis for the Mannesmann process model

The limited variation in the model results when the input parameters are changed is a good indication of the model stability.

Finite element model of buckle arrestors for deepwater linepipes

Deepwater pipelines are normally subjected to external pressure and bending and they are designed to prevent buckling and collapse failures. But a pipeline that is locally damaged may collapse and, if the hydrostatic pressure is high enough, the collapse may propagate along the

Figure 7:
FEM vs. experimental results for a flattening cross-over

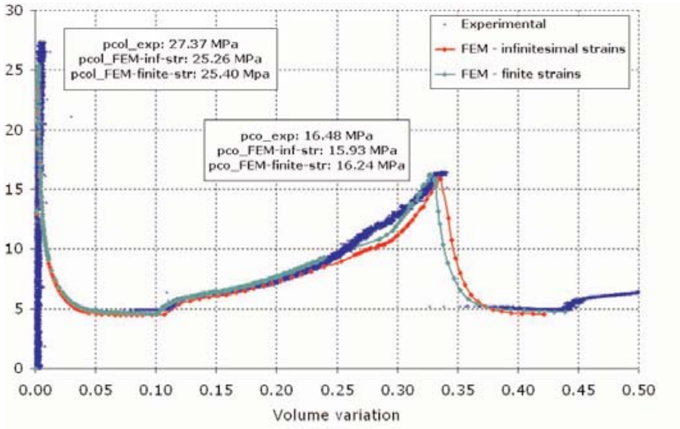


Figure 8:
Experimentally observed and FEM predicted shapes of collapsed pipes after a flattening cross-over

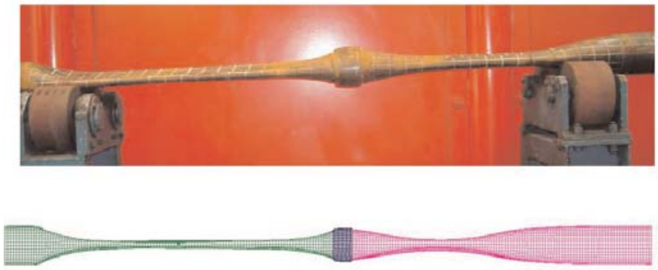


Figure 9:
FEM vs. experimental results for a flipping cross-over

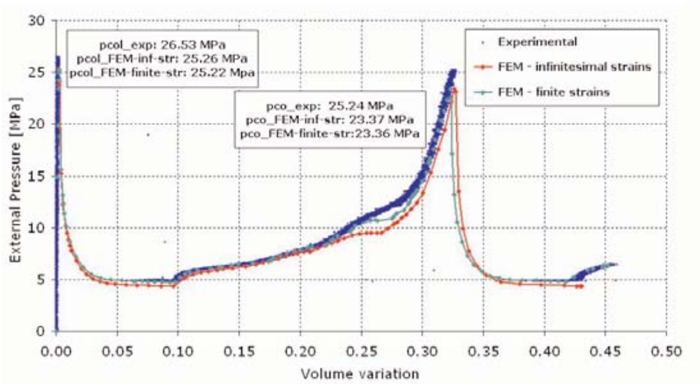


Figure 10:
Experimentally observed and FEM predicted shapes of collapsed pipes after a flipping cross-over

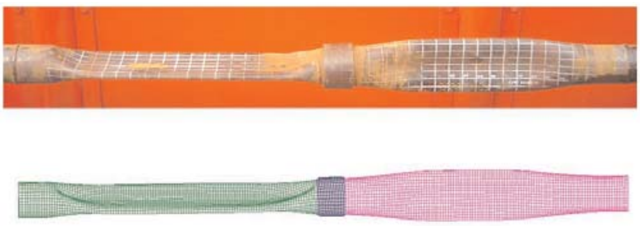


Figure 11:
Strain gages for verifying an OCTG connection model

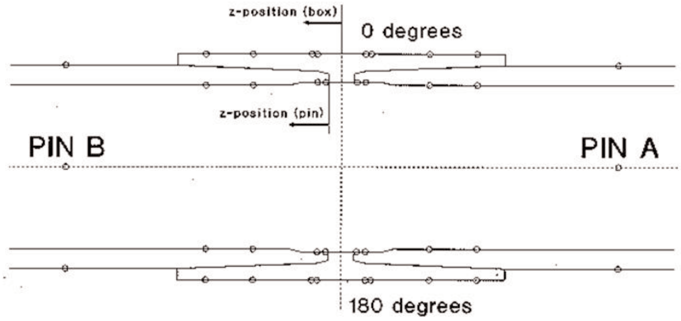


Figure 12:
Dope pressure measured during make-up

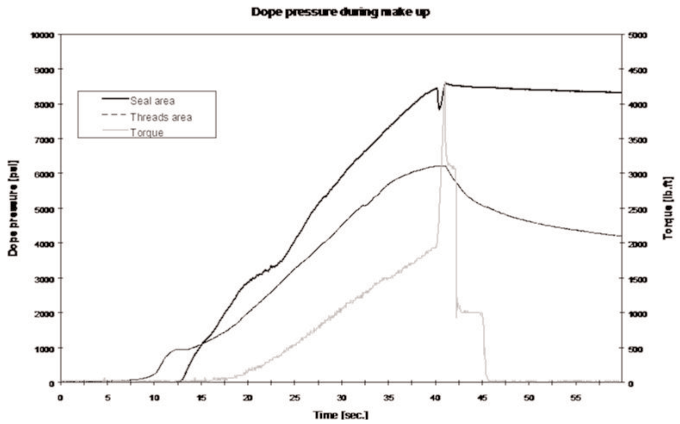


Figure 13:
Strains comparison without considering dope pressure in an over-doped connection.

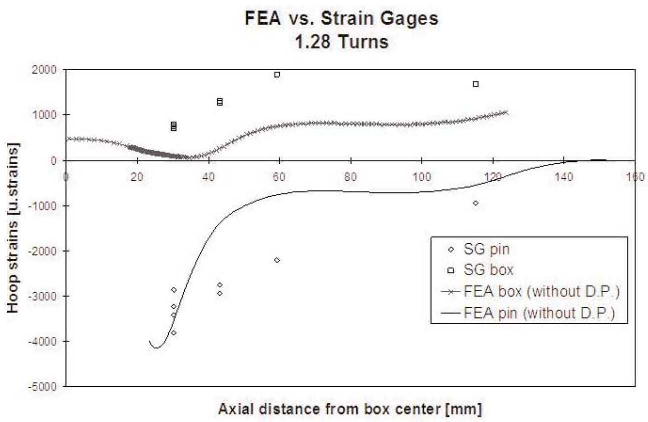
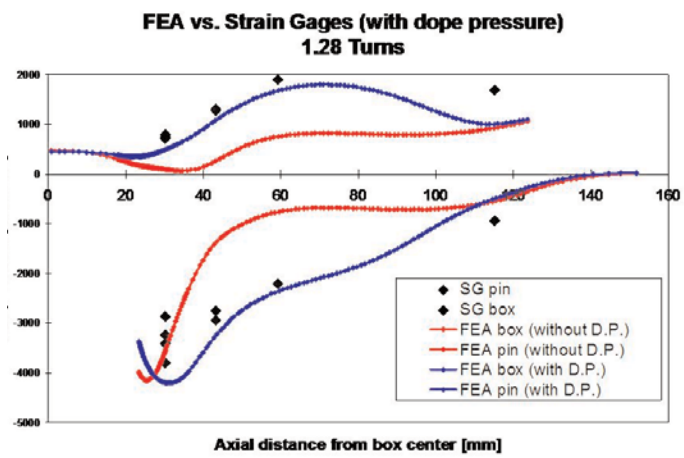


Figure 14:
Finite element analysis considering dope pressure.



pipeline. The collapse propagation pressure is the lowest pressure value that can sustain the collapse propagation [26]. Since the external collapse propagation pressure is quite low in comparison with the external collapse pressure, it is necessary to install buckle arrestors, at intervals along the pipeline, with the purpose of limiting the extent of damage to the pipeline by arresting the collapse propagation.

Buckle arrestors are devices that locally increase the bending stiffness of the pipe in the circumferential direction and therefore they provide an obstacle in the path of the propagating buckle; there are many different types of arrestors, but all of them typically take the form of thick-walled rings. The external pressure necessary for propagating the collapse pressure through the buckle arrestors is the collapse cross-over pressure.

In our paper [27] we focused on the analysis of the collapse and post-collapse behavior of pipelines reinforced with buckle arrestors: we developed finite element models to analyze the collapse, collapse propagation and cross-over pressures of reinforced pipes and we presented an experimental validation of the models. In particular we considered the case of welded integral arrestors.

Two different integral buckle arrestor cross-over mechanisms were identified in the literature: flattening and flipping. The occurrence of either cross-over mechanism is determined by the geometry of the pipes and of the arrestors [28].

In *Figs. 7-10* we present comparisons between numerical and experimental results for various [pipe –arrestor] configurations.

Finite strain or infinitesimal strain formulations?
In the post-buckling regime finite elastic-plastic strains are developed only at localized zones and therefore the analyst may doubt between using geometrically nonlinear finite strains (more expensive) or geometrically nonlinear infinitesimal strains (less expensive) models. Hence, in *Figs. 7 & 9* we compared the results provided by both models with the experimental results and we arrived to the conclusion that using the less expensive model is an adequate choice.

Finite element models of a threaded connection for OCTG: learning from validation

Oil country tubular goods are the pipes that go inside the oil wells for oil production (tubings and casings); their threaded connections have to be extremely reliable and provide adequate strength; also in many cases (proprietary connections) they must be gas-tight.

Nowadays finite element models are extensively used for the design of these threaded connections. Therefore the validation of these models is a very important issue [13, 29 and 30].

In *Fig. 11* we present the strain gages that we installed in an OCTG connection (pins and box). An actual connection was made-up with extra dope and the dope pressure values shown in *Fig. 12* were measured during the make-up. In *Fig. 13* we compare the strains determined via a standard finite element analysis with the strains measured in the full-scale test; it can be seen that the agreement between numerical and experimental values is not as good as in the cases reported in our previous publications. Then we re-run the analysis adding among the loads the dope pressure distribution determined in the full-scale test; in *Fig. 14* we compare the experimental results with the numerical results obtained with and without the inclusion of the dope pressure; it is obvious that the inclusion of the dope pressure improves the matching between the experimental and numerical results.

Engineering design considerations

As a result of the above discussed validation results, it was obvious that the over-doping condition should be always avoided and therefore the connection design was modified to include "dope pockets" that could allocate a possible amount of extra-dope without a pressure increase [31].

Conclusions

Finite element models are a powerful tool in industry for analyzing technological process. Since the reliability of the models is of utmost importance, the analyst should be able to make fundamental decisions regarding the mathematical model (modeling hypotheses), the numerical model (e.g. how many elements? and which elements?), numerical model inputs (e.g. material parameters).

After getting the results one should be able to verify the adequacy of the modeling hypotheses and of the discretization scheme. An experimental validation process is necessary to have reliable results that can be used in technological decisions.

The usage of black-boxes by analysts lacking the necessary background is a road map for disaster.

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