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# FINITE POINT METHOD SIMULATION TOOL TO SIMULATE AND IMPROVE POLYURETHANE FOAMING PROCESSES

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**SUMMARY**: FPM (Finite Point Method) mesh-free technology has been used to develop a module that enables to simulate and optimize the polyurethane foaming process. FPM is a mesh free method which does not require a 3D volume mesh, thus cutting model preparation time drastically. The software takes into account chemical reactions, provides access to the injection parameters like the number of filling gates, their area, the direction and the velocity of the injected liquids. Moving filling gates can be modeled in the case of open mold processes. The presence and location of the vents can be specified. The calibration methodology for the foam expansion law and numerical results for a demonstration case will be presented.

**KEYWORDS**: polyurethane foaming process, Finite Point Method (FPM), mesh-free calculations

## INTRODUCTION

### Industrial Needs

Polyurethane foams are widely used in many industrial applications, including automotive, upholstered furniture and mattresses, insulating panels for building and appliances. Depending on the desired application, polyurethane foams can be produced using many different chemicals and formulations. The physical properties of flexible polyurethane foams depend on their composition. They will be closely related to the characteristics of the polyol used, to the stoichiometry (polyol/isocyanate ratio) and to the water content (and so to the density). An accurate prediction of the polyurethane foaming process is of much importance notably for automotive parts especially dashboards, door panels, seat manufacturing. This involves the final quality of the product (monitoring the presence of

entrapped air pockets, homogeneity of the foam) and the structural resistance of this foam for crash and other structural applications (vibrations, acoustics, comfort, etc.).

FPM opens new possibilities in the design of the polyurethane foaming process, taking into account the physics of the chemical reactions and the real geometry. Therefore, choices regarding for example the mass of the reactants, the position and the movement of the filling gates can be made much earlier in the project loop. FPM is coupled with two structural codes that allow taking into account mould or structural deformation.

**Polyurethane Foams**

"*Polyurethanes are formed by reacting a polyol (an alcohol with more than two reactive hydroxyl groups per molecule) with a diisocyanate or a polymeric isocyanate in the presence of suitable catalysts and additives*." - Alliance of the Polyurethane Industry
Cellular or foamed PUs are manufactured by using blowing agents to form gas bubbles in the reaction mixture as it polymerizes. They are usually low boiling point liquids which are volatilized by the heat generated by the exothermic reaction between the isocyanate and polyol. Rigid foams yield sufficient exothermic heat from the reaction to allow foam expansion in association with the blowing agent. The foam which is produced is by two orders of magnitude larger in volume than the initial volume of the liquids which are mixed together. After mixing has occurred inside the tool, the foaming reaction takes usually around one minute to be completed.

**Chemical Reactions Involved in Polyurethane Foaming**

Foam expansion process is due to the chemical reactions involved after the mixing of the reactant liquids. This chemical reaction will create expansion of volume due to the production of carbon dioxide gas and polymerization. At the end, the foam is a heterogeneous material composed of a viscoelastic skin and a gas bubble.

The second reaction produces carbon dioxide gas in presence of water. In absence of water only a hard skin is obtained at the end of polymerization process without any volume expansion. The evolution of the concentration of the reactants will follow the evolution provided by the kinetics of the corresponding chemical reactions.

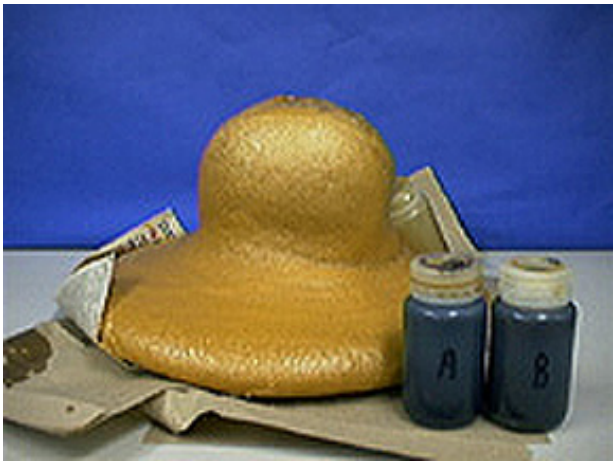



Fig. 1 Final shape of a polyurethane foam after mixing of products A (isocyanate) and B (polyol).

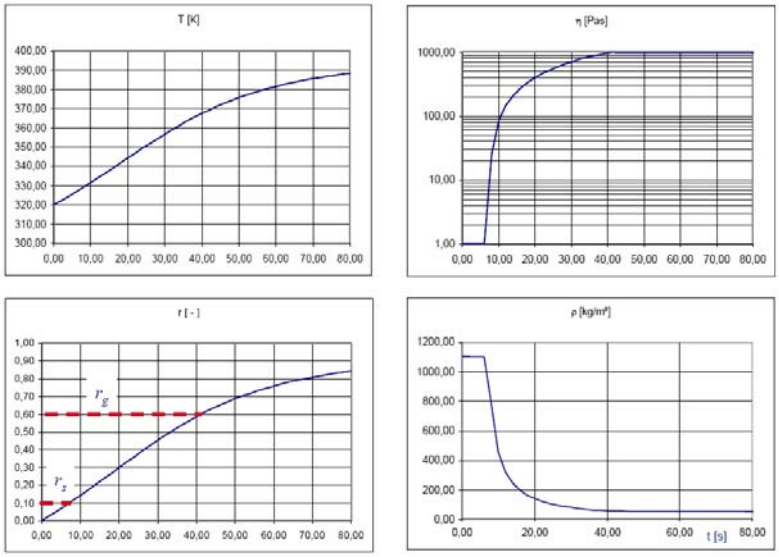



Fig. 2 Evolution of temperature, viscosity, reaction rate and density during the expansion process.

**FPM Fluid Code**

FPM is an innovative mesh-free thermal CFD code for incompressible and compressible flows. FPM includes Newtonian or non-Newtonian viscosity laws, natural convection, heat conduction, heat exchange at the boundaries. The numerical scheme and the theoretical background are described in ref. [3], [4], [9] and [10]. FPM is coupled with structural mechanics code so that the deformation of the mould if any can be represented. The method is widely used in the field of airbag deployment in car industry for the simulation of compressible gas flow inside airbags. Here, the membrane (or boundary) of the airbag changes very rapidly in time and takes a quite complicated shape, see Ref [5] (Kuhnert et al., 2000).

[1] $R-N=C=O+R'-OH \rightarrow R-NH-CO-O-R'$

[2] $H_2O+2R-N=C=O \rightarrow CO_2+R-NH-C-NH-R$

Fig. 3 Example of chemical reactions during PU foaming process.

$$d/dt\left(\frac{[OH]}{([NCO]_0+[OH]_0)}\right)=-K1(T)\left(\frac{[NCO]}{([NCO]_0+[OH]_0)}\right)\left(\frac{[OH]}{([NCO]_0+[OH]_0)}\right)$$

$$d/dt\left(\frac{[H2O]}{([NCO]_0+[OH]_0)}\right)=-K2(T)\left(\frac{[NCO]}{([NCO]_0+[H2O]_0)}\right)^2\left(\frac{[OH]}{([NCO]_0+[H2O]_0)}\right)$$

*[NCO]: NCO concentration in mol/m3, $NCO_0$ is the initial concentration*

*[OH ]: OH concentration* *[H20] : H20 concentration*

*T: temperature* *K1, K2: temperature dependent kinetic constants*

Fig. 4 Kinetics of the chemical reactions.

**Demonstration Case**

The geometry is presented below. The two liquids (isocyanate and polyol) are mixed and injected from the lower filling gate at a velocity of 1 m/s during 2 s. The mixture ratio between isocyanate and polyol is taken in this case at 68%.

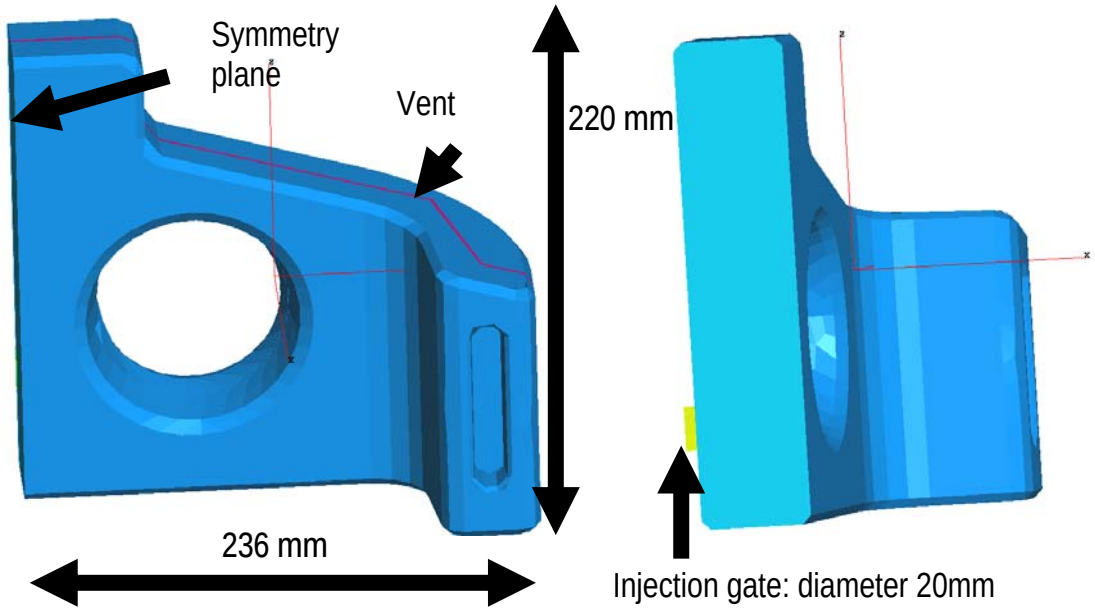


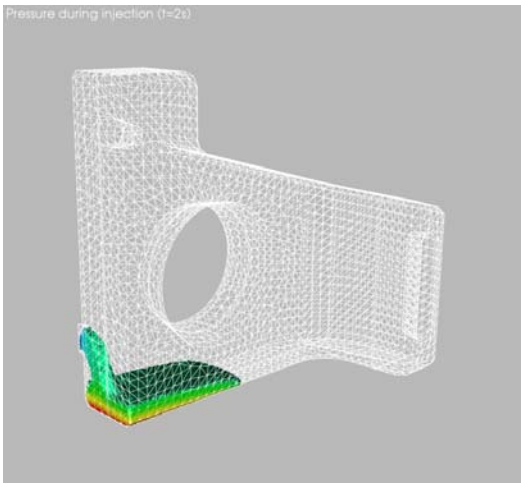

Fig. 5 Half geometry of the demonstration case.

The total volume to be filled is 1.85 liter. Before expansion starts, the volume of the foam, still in its liquid phase, is 0.115 liter. The mold surface is taken at room temperature, 320°K and remains isothermal during the foaming process. Nevertheless the internal temperature of the foam will rise due to the heat production of the chemical reaction. It is possible to define a heat exchange coefficient between the mold surface and the foam if required.

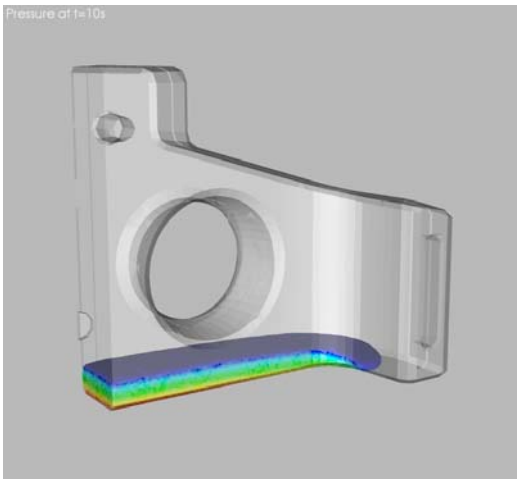
The maximum expansion (ratio between the initial and the final densities) is around 19. Viscosity starts at 1 Pa.s after the mixing of the two liquids and grows up to 1000 Pa.s (arbitrary high value) at the end of the foaming process. Fig. 6 shows the different stages of the expansion process till 40 s, it displays the contours of total pressure (in blue: low pressures; in red: high pressures). The effects of the increasing viscosity are visible.

## CONCLUSION

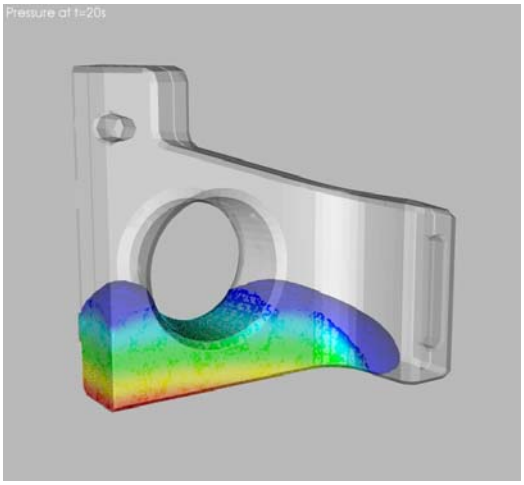
The first prototype of FPM is currently being validated through industrial joint projects on medium and large scale models covering a wide range of applications. An intrinsic model based upon the chemical reactions has been proposed. This model is defined by the user in the model input and can be adapted for any specific need. FPM as a mesh free code is very well adapted in several ways for dealing with foam expansion : very precise modeling (and at a reasonable cost) of the foaming front, non Newtonian viscous models, temperature effects, coupling with structural mechanics and above this no need to create a volume mesh which can save considerable amount of time for model preparation.



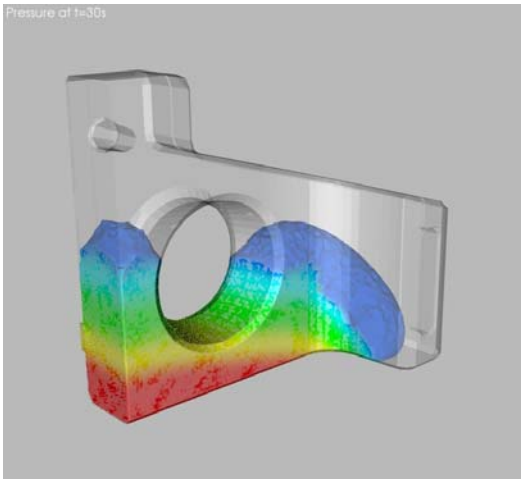

T = 2 s (during the injection process)



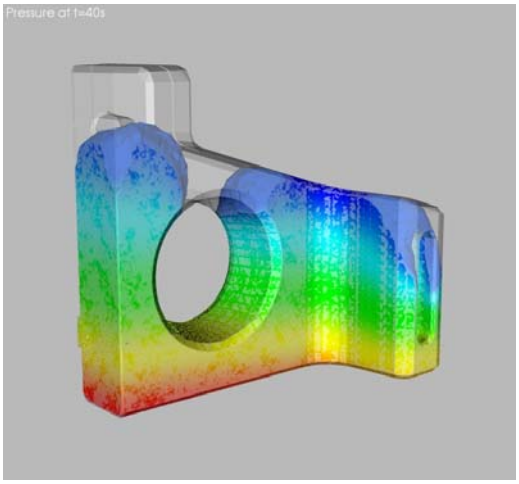

T = 10 s (expansion starts)




T = 20 s




T = 30 s




T = 40 s

Fig. 6 Pressure contours during the expansion process.

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