SIMULATION OF GLASS PROCESSES WITH POLYFLOW, A FINITE ELEMENT PROGRAM

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Polyflow is a general Computational Fluid Dynamics finite element program which simulates the flow of Newtonian and non-Newtonian fluids, with a special emphasis on rheological complex liquids in industrial processes.
A major objective of Polyflow is Computer Aided Processing: using the computer as a laboratory, the engineer understands, modifies, creates, tests and improves processes in which flow of viscous liquids plays a dominant role. The code is used for modeling a variety of processes: extrusion, fiber spinning, laminar mixing, coating, sedimentation, heat transfer, chemical reactions, flow through channels, thermoconvection and many others. Advanced computational methods have been implemented for calculating free surfaces and interfaces which are typical of many processes. Polyflow is also used as a toolbox for developing new applications.
The specificity of the numerical methods (finite element, direct solver), the original physical modeling of glass processes and the ability of solving a wide class of thermal, flow and deformation problems will be the main topics of this presentation.

GENERAL SPECIFICATIONS

Polyflow solves the flow of isothermal and non-isothermal generalized Newtonian and viscoelastic fluids, the flow of viscous fluids through porous media and flows and reactions related to chemical vapor deposition [1]. Several types of materials separated by interfaces can co-exist in the flow domain. A typical example of such "multi-domain" calculation is the combined study of melting tank and refractory walls. Rather than imposing a measured - generally inaccurate - value of the heat loss at the furnace boundaries, this technique allows imposition of a room temperature at the external faces of the refractories. The additional computational cost is that of a heat exchange problem in a solid.

All steady-state non-linear problems are calculated with Newton's method; solutions to highly non-linear problems can be reached by means of the versatile "evolution" algorithm implemented in Polyflow. To reach a steady-state simulation of thermoconvection in a glass melting tank, increasing gravity values of decreasing conductivity values are used in this automatic procedure. Starting from an "easy", quasi-linear situation, the calculations automatically advance to solve an increasingly non-linear problem to reach the final values of the required simulation.

On the other hand, time dependent problems are solved with a fully coupled implicit method which guarantees stability; the time step is automatically adjusted to satisfy a required accuracy.

Polyflow calculates free surfaces and interfaces in 2-D and 3-D; such calculations are fully implicit and solved with Newton's method. Free surface problems require a remeshing technique on the flow domain. Polyflow contains a library of remeshing techniques of the algebraic and of the elliptic types.

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Polyflow contains a wide library of finite elements. Although default selections are available for all flows, the user can easily request other types of interpolations. In particular, sub-refinement is available as well as non-uniform discretization. Solving a high-Péclet and low-Reynolds glass convection problem usually requires much more degrees of freedom for temperature than for velocity. For this reason, higher order shape functions can be chosen for the temperature field whereas ordinary linear shape functions are selected for velocity. This non-uniform discretization technique significantly reduces the computational cost without affecting the global accuracy and will be intensively used for glass convection simulations.

The present paper presents three application domains of Polyflow for glass processes: 1. the TC 21 test-case; 2. specific physical modelling of bubbling, boosting and radiative correction and 3. other glass-related processes like fiber spinning or blow molding.

TC 21*) TEST CASE

Benchmarks

The TC 21 benchmark consists in the numerical simulation of velocity and temperature fields in a small idealized tank furnace [5]. Given temperature and velocity boundary conditions - temperature profile at the surface and throat outflow - generate recirculation cells in the glass volume. The numerical simulation of the four different versions of this benchmark was realized by Polyflow without any difficulty as the problem was simply posed in terms of thermoconvective flow. In comparison with other classical numerical methods (finite differences and finite volumes spatial discretization, iterative solver), some major differences have to be pointed out.

As mentioned before, the solver of Polyflow is a *fully coupled direct method.* To reach the final set of physical values characterizing the TC 21 benchmarks, 10 steps of increasing non-linearity were necessary and, for each step, ca. 5 iterations of Newton's scheme were required to reach convergence.

The second particularity lies in the spatial discretization; the high Prandtl number value indicates the predominance of advection in the temperature equation. Therefore, in the library of the available elements, *quadratic temperature and linear velocity* finite elements were selected. The number of degrees of freedom for temperature is then increased while the velocity unknowns are represented by lower order interpolation.

Finally, a moderate number of elements was requested for a given level of accuracy (measured by the heat balance). Typical values of $28 \times 8 \times 6$ elements grid results in a ≈ 5 % heat balance. These values are to be compared with the grid points used by uniform low-order methods, typically $35 \times 10 \times 6$. The full simulation requires about 20 CPU hours on a Silicon Graphics Personal Iris Workstation.

Unsteady TC 21 test case

While the numerical solution of the TC 21 benchmarks does not require any additional physical modeling, we exploited the Polyflow capacities to simulate two unsteady situations for the TC 21 test case [3].

1. The first study is the unsteady simulation of sudden modification of boundary conditions (10% increase of the pull, 5 °C decrease of the temperature profile at the surface, . . .). The time discretization algorithm used in Polyflow allows for the automatic selection of the time step and clearly indicates both temperature and velocity time evolutions. Variations of conductivity show the influence of this parameter on the thermal time constants while velocity evolutions were apparently unaffected.
2. The second unsteady situation consists in the mixing modeling. When operating an industrial furnace, changes of glass do not occur in the whole domain, but an unsteady mixing is realized. Low diffusion coefficient - leading to high "mixing Péclet" number - were selected and showed the accuracy of numerical resolutions. It should be noted that the concentration is not the result of a tracking calculation but another global variable added to the set of partial differential equations. Residence time calculations realized with Polyflow consist also in the resolution of a new problem defined on the whole thermoconvective domain.

GLASS MELTING FURNACE MODELLING

Industrial furnaces significantly differ from the idealized benchmark of the TC 21. To simulate accurately realistic furnaces, different physical models are presently developed in addition to the basic thermoconvective model flow solver.

Electrical heating

The numerical treatment of electrical heating does not present great difficulties. Under classical assumptions the electrical potential field is governed by a Laplace equation. The polyflow capabilities of simulating the unsteady electrical boosting has been demonstrated [5]. The correction of the Lorentz force is also possible and leads to an accurate description of the molten glass velocity in the vicinity of the electrodes [4].

*) 21 st Technical Committee of the International Commission on Glass "Modelling of glass melt"

In most applications the engineer wishes to impose a given current intensity rather than potential difference between electrodes. This problem belongs to the set of commonly called "inverse problems". A numerical technique is implemented in Polyflow to solve the inverse problems. This method, based on generalized Lagrangian multipliers, avoids classical trial and errors outer iterations on the unknown values and solve the inverse problems at nearly the same cost as that of the direct problem. The inverse method is also useful for electrical heating simulations where connections between electrodes impose equalities of currents and/or potentials.

Radiative correction

The importance of internal radiation in the glass melts is well known. The Rosseland approximation appears to be the only practical model that can be used for realistic 3-D simulations. However, the Rosseland diffusion approximation is unable to take into account the sudden modification of the temperature gradients at the boundary, the so-called "radiation slip" [5]. This temperature difference significantly modifies the amplitude of the thermoconvection in the whole domain. Radiative boundary conditions including the correction to the Rosseland model are proposed in Polyflow, they simulate the radiation slip and provide accurate thermal boundary conditions for the thermoconvective problem. Figure 1 illustrates the principle of radiative correction: a given temperature T_1 is to be imposed at the wall while the effective numerical boundary condition should rather impose the T_x value such that the correct temperature level is reached in the domain. The relationship between T_1 and T_x involves the values of the wall emissivity and the medium absorptivity and conductivity.

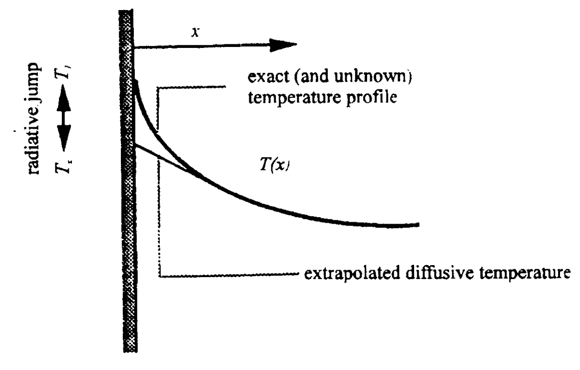

Figure 1. Radiative slip boundary condition.

Bubbling

Air bubbles have become an integral part of glass melting tank design. The numerical simulation of bubbling can follow two different ways: a local description of the bubble trajectory or the global expression of the force exerted by the series of bubble on the convective flow. The Polyflow bubbling simulation consist of an additional force term expressing the global coupling between the bubble stream and the velocity of the molten glass [6]. With that global model, the simulation of bubbling can be realized with a negligible additional CPU cost.

OTHER GLASS PROCESSES

To illustrate the open capacities of Polyflow, the numerical simulation of two processes related to the glass industry is finally presented.

Fiber spinning

The production of synthetic fibers is a delicate process associated with severe technological requirements. Fiber spinning is characterized by a non-isothermal nature of the flow which, as in the case of polymer melts, is dominated by its extensional behavior. On the basis of the spinneret and the material properties of the fluid, the numerical simulation supplies the geometry of the drawn fiber, the temperature and the stress field together with the relationship between the draw ratio and the axial force exerted on the filament.

Polyflow provides the user with all the necessary ingredients for the successful simulation of fiber spinning: a wide class of viscoelastic models, an accurate calculation of free surfaces including the effect of surface tension, the coupled calculation of heat transfer in the melt and in the die and, finally, special elements for high Péclet number flows. Numerical simulation therefore complements experimentation for a quicker adjustment of the manufacturing process.

Blow molding

Blow Molding is a standard process for the mass production of hollow objects. The products may be simple, such as axisymmetric bottles, or have a complex three-dimensional shape, such as gas tanks of large dimension. The numerical simulation of blow molding requires an accurate description of a flowing body with large non-isothermal deformations; the external free surface is constrained by contact with the wall.

An original remeshing technique has been implemented in Polyflow for handling the large deformations of a thin fluid shell, while a robust geometrical algorithm has been developed for detecting contacts between the fluid and the wall of the mold. Since the final thickness is a critical factor for the quality of blown products, tracking of material lines is used for establishing a relationship between the parison thickness and the thickness distribution of the blown product.

Figure 2 shows a combined extrusion-blow molding simulation. Remeshing, moving boundaries, free surfaces, material lines tracking and contact lines are some of the numerical tools used for this industrial simulation.

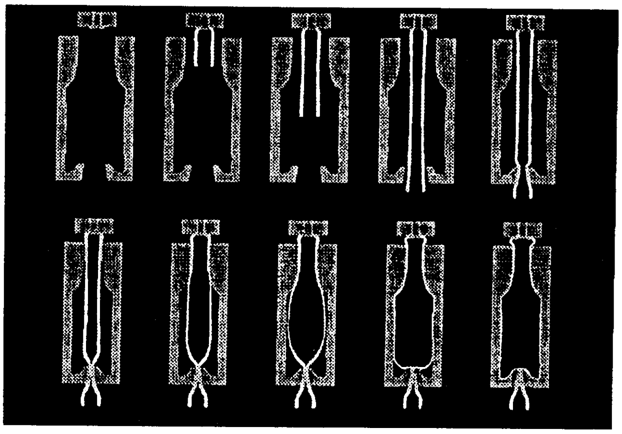

Figure 2. Combined Extrusion-Blow Molding Simulation.

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MODELOVÁNÍ TAVÍCÍCH SKLÁŘSKÝCH PROCESŮ POMOCÍ PROGRAMU POLYFLOW

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Polyflow je obecný výpočetní program dynamiky kapalin založený na konečných prvcích a modelující tok newtonských a nenewtonských kapalin, zvláště vhodný pro reologicky složité tekutiny vyskytující se v průmyslových procesech.

Hlavním cílem programu Polyflow je počítačem podporované řízení průmyslových procesů; technolog využívající počítač jako laboratoř má být schopen pochopit, upravovat, vytvořit, odzkoušet a zlepšovat procesy, ve kterých hraje dominantní roli proudění. Program nachází uplatnění v nejrůznějších průmyslových procesech, jako jsou například vytlačování, tkaní vláken, laminární mísení, nanášení povlaků, sedimentace, přenos tepla, chemické reakce, průtok potrubím, konvekce tepla, a mnohé další. Moderní výpočtové metody jsou využívány pro výpočet volných povrchů a rozhraní, typických pro větší počet procesů. Polyflow se rovněž využívá jako nástroj pro vývoj nových aplikací. V tomto příspěvku jsou hlavními tématy specifika numerických metod (konečný prvek, přímá metoda řešení - direct solver), původní fyzikální modelování procesů tavení skla, a možnost řešení nejrůznějších problémů v oblastech přenosu tepla, proudění a deformací.