Computers and Mathematics with Applications 68 (2014) 27–43

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Free boundary problems and optimal control of axisymmetric polymer crystallization processes

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ARTICLE INFO

Article history:
Received 2 November 2013
Received in revised form 22 April 2014
Accepted 3 May 2014
Available online 22 May 2014

Keywords:
Stefan problem
Optimal control
Polymer crystallization
Axisymmetric geometry
Numerical simulations

ABSTRACT

The non-isothermal crystallization of a hollow cylindrical polymer sample with radial symmetry is studied. Three radial cooling strategies are considered: cooling from inside (outward cooling), cooling from outside (inward cooling), and cooling from both sides (double cooling). When the initial and boundary conditions are axisymmetric, the crystallization problem can be reduced to a one-dimensional formulation where a free boundary problem framework can be used. The solution is approximated by appropriate one-phase Stefan problems for which the analytical solution is provided. These results are compared to direct numerical simulations of the crystallization process, finding an excellent agreement in the approximation of the time-evolution of the crystallization front, the temperature distribution and the crystallization time. In a second part, the corresponding optimal control problems are formulated for a cost functional assessing the use of low temperatures and the duration of the crystallization process. Analytical expressions of the approximated optimal controls are derived for each cooling strategy. In particular, the double cooling case presents special difficulties that we are able to overcome by extending the technique that we previously developed for the case of homogeneous rectangular samples.

1. Introduction

Designing the optimal cooling strategy is a core problem in polymer crystallization [1]. As an industrial material manufacture process, the main requirements of polymer production industry are the reduction of the processing time and the restriction of the use of excessively low cooling temperatures, which are very expensive to reach and to maintain. These two interests compete with each other: shortening the duration requires low temperatures, and avoiding low temperatures makes the duration longer. Of great interest for industry is thus to find the optimal control of the cooling temperature applied to the polymer melt which balances the production costs.

In rectangular samples with spatially homogeneous cooling objects, the optimal applied temperature has been found for the two possible cooling strategies: double cooling, when both sides of the sample are cooled under the critical freezing threshold, and single cooling, when only one side of the sample is cooled (and a zero-flux boundary condition is used at the other side). In both cases, the optimal cooling strategy consists in applying a constant temperature, the same one at both ends in the double cooling case [2,3]. This study was performed by reducing the rectangular problem to a one-dimensional

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http://dx.doi.org/10.1016/j.camwa.2014.05.003
0898-1221/

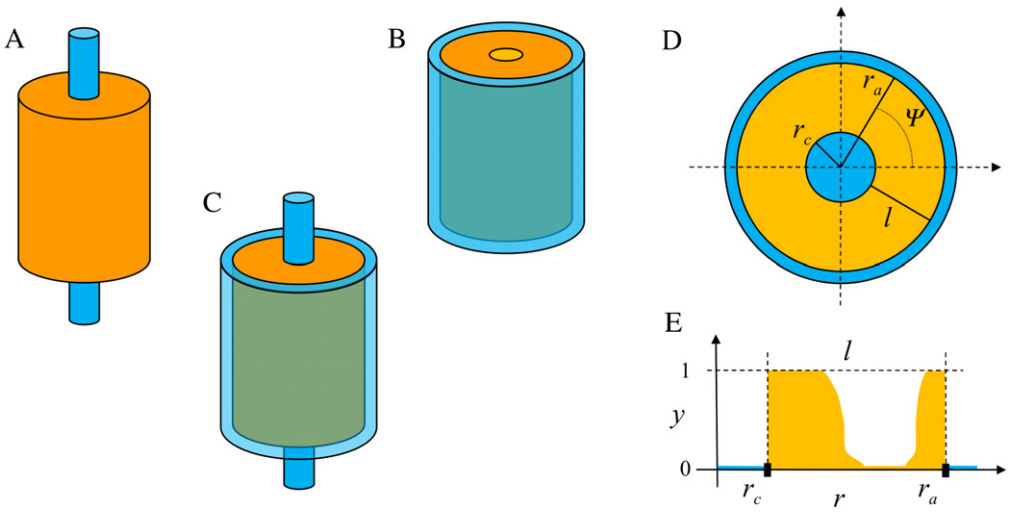

Fig. 1. From cylindrical geometries to the axisymmetric one-dimensional formulation, using thermally homogeneous cooling objects. (A) Outward cooling, (B) inward cooling, (C) double cooling, (D) radial symmetry, (E) crystallinity $y(r, t)$ as a one-dimensional spatial function of the radius r at a time t in the double cooling case.

(1D) problem, on the basis of the spatial homogeneity of the material and the boundary and initial conditions. There, the crystallization process is described by identifying the region where crystallization takes place with a moving free boundary. A free boundary problem (FBP) framework, presented in [4], allowed us to derive analytical approximations of the temperature field and the time-evolution of the position of the crystallization front, as well as important magnitudes such as the duration of the crystallization process.

Predicting cooling duration and temperature field are critical for maintaining optimum productivity costs [5]. The question arises as to whether the efficiency can be improved by using higher dimensional geometries (e.g. two-dimensional samples with axial symmetry, two-dimensional rectangular samples with inner contacts, etc.). A natural extension of one-dimensional studies consists in considering cylindrical samples, as they can take profit of the radial nature of heat transfer in two dimensions. Cylindrical samples are indeed used in polymer crystallization [1,5,6]. On the other hand, cylindrical samples are of particular interest from the mathematical viewpoint, due to the fact that, in the case of axial symmetry, they lead to one-dimensional problems.

The present paper extends these previous studies to the case of cylindrical samples in which a hollow cylinder of internal radius $r_c > 0$ and external radius $r_a > r_c$ is cooled under its critical freezing value T_f. The three possible strategies are considered: the *outward cooling* strategy, which consists in applying a cooling cylindrical object of radius r_c to the interior of the sample, the *inward cooling* strategy, where the sample is cooled from outside with a larger hollow cylinder of inner radius r_a and outer radius larger than r_a, and the *double cooling* strategy, which consists in combining both strategies. See Fig. 1. In each case, the temperature of the cooling objects is considered time-dependent and denoted by $u_c(t)$ and/or $u_a(t)$, according to the side(s) of the sample to which the corresponding cooling object is applied. For simplicity, the cooling objects are assumed thermally homogeneous so that there is no spatial variation in the applied temperature with respect to the vertical z-axis and the angular coordinate (azimuth) ψ. Uniformity along the z-axis and radial symmetry are also assumed for the rest of the parameters and the boundary and initial conditions. The resulting geometry allows then to reformulate the problem as a 1D problem for the radial spatial variable $r \in [r_c, r_a]$. The emergence of a crystallization front is expected, which will allow us to use the FBP framework.

The model consists of two non-linear partial differential equations for the degree of crystallinity $y(r, t)$, defined as the mean volume fraction of the space occupied by crystals, and the temperature field $T(r, t)$, coupled by means of the rate functions of nucleation and growth $b_N(T)$ and $b_G(T)$, the function of starting of nucleation $\kappa(y) = (1-y)^2$, and the function of aggregation and saturation of nuclei $\beta(y) = y(1-y)$:

$$y_t(r, t) = \beta(y(r, t))b_G(T(r, t)) + v_0\kappa(y(r, t))b_N(T(r, t)), \tag{1}$$

$$T_t(r, t) = \sigma\left(T_{rr}(r, t) + \frac{1}{r}T_r(r, t)\right) + a_G\beta(y(r, t))b_G(T(r, t)), \tag{2}$$

for $(r, t) \in (r_c, r_a) \times (0, \tau)$, where τ is the time at which the cooling process is stopped. Subindexes t and r in y_t, T_t, T_r and T_{rr} denote first-order (resp. second-order) partial derivative with respect to the corresponding variable t or r. Let us stress that the heat operator is expressed here in polar coordinates and that the term depending on the angular coordinate ψ does not appear in Eq. (2) because the boundary and initial data are also axisymmetric. The spatial lengths are defined as $l = r_a - r_c$, the radial length of the sample, and l_z, the height of the sample along the z-axis. This model was originally introduced by Capasso in [7] (see also [1]).