International Journal of Heat and Mass Transfer 98 (2016) 176–182

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

Numerical study of gas mixture separation in curved nozzles

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ARTICLE INFO

Article history:
Received 29 October 2015
Received in revised form 11 February 2016
Accepted 4 March 2016

Keywords:
Curved nozzle
Species separation
Supersonic flow
Separative capacity

ABSTRACT

Species separation can be produced by imposing a pressure gradient in gaseous mixtures, which induces different molecular velocities depending on the molar weight. Pressure gradients can be achieved by centrifugal forces brought about by the passage of the gas through a curved nozzle at supersonic velocity. The efficiency of this process depends on the geometry of the nozzle as well as the flow operating conditions. The numerical solver Fluent was used in order to produce a model of the aerodynamics and the oxygen diffusion of a steady-state flow of air in a curved nozzle. The development of the pressure and O_2 concentration profiles along the nozzle were analyzed for different pressure boundary conditions at the inlet and the exit, testing several nozzle sizes. Optimum values of the cut and the inlet pressure were found which maximize the separation efficiency. The effect of the exit pressure was associated with the axial pressure distribution along the inner wall of the nozzle. The results were compared with measurements showing good agreement.

1. Introduction

It is well known that species separation can be produced by imposing a pressure gradient in gaseous mixtures, which induces different molecular velocities depending on the molar weight. A direct method to produce pressure gradients are centrifugal forces, which can be brought about by the passage of the gas through curved nozzles. This kind of processes are known as fixed-wall centrifuges, in contrast with the so-called centrifuge process, and have been widely studied in the 60's and 70's [1–4]. According to Stern et al. [5] the earliest proposal of separating gas mixtures in high velocity jets go back to P. Dirac during World War II and the concept was experimentally verified by Tahourdin in 1946. To the authors' knowledge, the first quantitative model of the process was presented by Sherman [6], where the mass diffusion in an aerodynamic field is separated in terms of concentration, pressure and temperature gradients, and volume forces.

Becker et al. [2] found that the optimum operating conditions of curved nozzles of different sizes leave approximately invariant the product of the inlet pressure times the diameter. Further pressure and size effects are also discussed in [1]. Similar scaling laws were suggested for free jets in which strong local pressure gradients are also generated by strongly curved streamlines [8–10]. In some of these systems, the experimental conditions extend to the free molecular regime, which invalidate the aerodynamic description. Molecular separation features of this regime, called Mach number focusing, are discussed in [11]. Li et al. [12] proposed that the aerodynamic separation of species can be enhanced by the formation of clusters. To model such cases, the continuum mechanical description should be complemented by appropriate particle descriptions.

Recently, there has been a renewed interest to use the current computational capabilities in gas separation processes of multicomponent flows [13–15], including laser assisted aerodynamics [26]. For curved nozzles, the numerical modeling has been proposed in the 80's by Vercelli [7] who used a finite difference scheme to solve the isotopic separation of UF_6; but otherwise there are no further reports in the open literature. In the present article a numerical model of the aerodynamics and the oxygen diffusion of a steady-state flow of air in a curved nozzle is presented. The solver Ansys Fluent [16,17] is used to implement the aerodynamic equations to calculate the velocity, pressure and temperature fields, and also the mass diffusion between nitrogen and oxygen. The results are compared with experimental measurements showing good agreement. Finally the development of the pressure and O_2 concentration profiles along the nozzle for different boundary conditions at the inlet and the exit, for several nozzle sizes, is analyzed to identify scale effects.

2. Experimental setup

In order to have a reference to compare with, an experimental test nozzle designed to operate with air at low pressure conditions

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.03.015
0017-9310/

was constructed. Figs. 1 and 2 show a photograph of the nozzle and a diagram of the experimental setup. The outlet flows Q_L and Q_P discharge in a single buffer chamber which is vacuumed by means of a Root mechanical pump at a flow rate of 210 m^3/h. The outlet pressure P_b (2.0 ± 0.1 mbar) is measured before the buffer with a pirani-gauge type manometer. The inlet pressure P_o (52 ± 1 mbar) is measured by a capacitive absolute manometer and it is controlled by tuning valve A.

To determine the change in concentration of oxygen and nitrogen, gas samples are collected from the inlet flow and the outlet flow Q_L, which is depleted in oxygen. The samples are stored in a flexible vessel containing approximately 5000 cc at ambient pressure. The oxygen concentration of each sample is measured with an electrochemical analyzer Siemens ULTRAMT 23. The experiment was repeated three times, obtaining an average depletion in oxygen of (0.10 ± 0.01)%. The results are shown in Table 1.

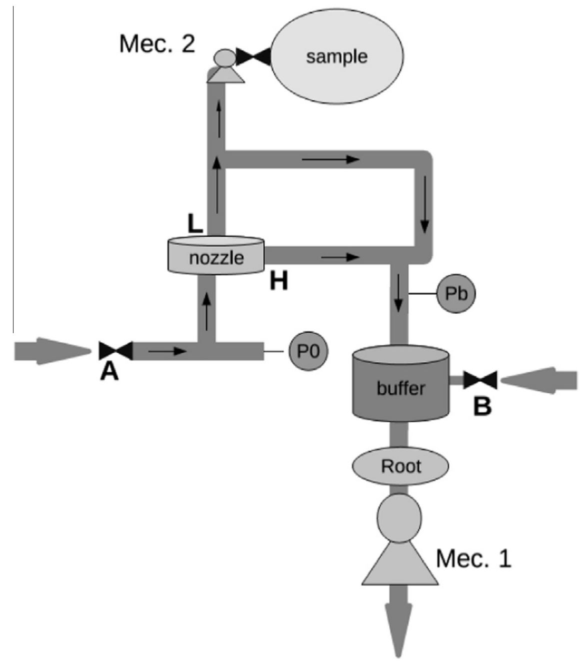

Fig. 2. Diagram of the experimental setup.

Table 1
Measured oxygen concentration.

Sample	Inlet (%)	Outlet (Q_L) (%)
1	20.98	20.89
2	20.92	20.83
3	21.01	20.92

3. Numerical model

The aerodynamics of the nozzle was modeled using a 2D approximation neglecting the effects of the lateral walls. The inner curved wall is described by a circular arc of radius 7.2 mm, whose center is taken as the origin of coordinates. The external wall is described by a circular arc of radius 10.4 mm centered at the point (1.4 mm, 0.7 mm). A mesh of 3858 quadrilaterals was taken as the base reference, which then was subsequently refined to ensure numerical convergence (Fig. 3). The minimum orthogonal quality and the maximum aspect ratio of the meshes, determined using the capabilities of the software [20], are listed in Table 2.

The equations of compressible fluid in stationary state were numerically solved with the code Ansys-Fluent, which is based in the finite volume method with the gas density taken as an independent variable within the flux-difference-splitting scheme [18,19]. Turbulence models were not included because the residence time of the fluid through the process is not enough to trigger this regime.

The mean molecular mass of the air was taken as 28.97 g/mol. A linear dependence with the temperature was assumed for the thermal conductivity. The temperature dependence of viscosity and specific heat was taken from the data provided by the solver. The functions were compared with the experimental data reported by Bergman et al. [20] showing good agreement (Fig. 4). Constant pressure boundary conditions were imposed at the inlet and the outlets, although the exit pressure is used only when the exit flow is subsonic. At the curved walls null velocity and constant temperature conditions are imposed.

The convergence of the numerical calculation was tested increasing the refinement of the mesh. Fig. 5 shows the evolution of the residual errors relative to the initial condition for each mesh detailed in Table 2. It can be seen that the final error, $<10^{-13}$, is the same in all cases. Moreover, the number of iterations required to achieve convergence increases with the square root of the mesh size, which is consistent with the finite volume method.

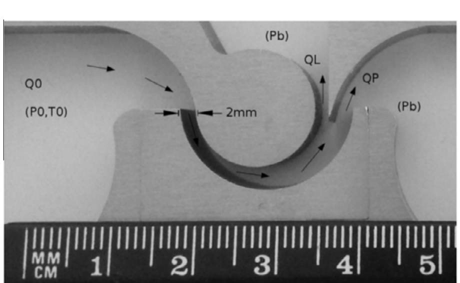

Fig. 1. Photograph of the curved nozzle showing the inlet flow rate Q_o, the inlet and exit pressures P_o and P_b, the inlet temperature T_o, exit flow rates Q_L and Q_P.

The solution of the aerodynamic problem provides the mechanical and thermal fields, *i.e.*, velocity, pressure and temperature, which controls the diffusion between species. In the absence of external forces such as electromagnetic fields, the diffusion between gas species is driven by concentration, pressure and temperature gradients. The diffusion velocity between species is then given by [21]:

$$u_1 - u_2 = -\frac{n^2}{n_1 n_2} D_{12}\left[\nabla c_1 + \frac{n_1 n_2 (m_1 - m_2)}{n\rho}\frac{\nabla P}{P} + k_T \frac{\nabla T}{T}\right] \quad (1)$$

where n_i, u_i and m_i are the number density, relative velocity respect to the average velocity of the mixture, and molecular mass of the species i, D_{12} is the diffusion coefficient, and:

$$n = n_1 + n_2 \quad (2)$$

$$\rho = n_1 m_1 + n_2 m_2 \quad (3)$$

Assuming a reference frame moving with the mean velocity of the mixture, u_1 and u_2 satisfy:

$$n_1 u_1 + n_2 u_2 = 0 \quad (4)$$

The diffusion flux of oxygen, $J_1^D = n_1 u_1$, is then given by:

$$J_1^D = -n D_{12}\left[\nabla c_1 + \frac{n_1 n_2 (m_1 - m_2)}{n\rho}\frac{\nabla P}{P} + k_T \frac{\nabla T}{T}\right] \quad (5)$$

In the laboratory reference frame the total flux of oxygen J_1 is given by: