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The driving force distribution for minimum lost work in chemical reactors close to and far from equilibrium. I. Theory

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October 13, 1999

Abstract

We present a mathematical procedure for determination of the driving force distribution in a chemical reactor that has minimum lost work for a given production rate. It is shown how the path of minimum lost work is determined from knowlegde of reaction kinetics, using the reaction $A \to B$ as an example. The normal chemical reaction has a non-linear relation between the rate, r, and the driving force, $-\frac{A}{T}$, where A is the affinity and T is the absolute temperature. Minimum lost work is obtained when $\frac{A}{T} + r d(\frac{A}{T})/dr$ is constant. This criterion is converted into a more practical criterion for the operating temperature along the reactor. The inverse operating temperature should be parallell to the inverse equilibrium temperature, when the enthalpy of reaction is constant.

1   Introduction

Chemical reactors are normally designed to operate at maximum reaction rate, see e.g. [4]. In this article, we shall study another reactor path, namely the path that looses minimum of useful work. The lost work per unit time (from now on called only the lost work) in a chemical reactor is given by the Gouy-Stodola theorem (see e.g. [1]):

$$W_{lost} = T_o \Omega \int \sigma dx \tag{1}$$

where σ is the entropy production rate per unit volume. The reaction takes place at temperature T, but the lost work is referred to the temperature of the surroundings, T_o. The lost work is obtained by integrating the entropy production rate per unit volume over the reactor volume. For simplicity we used a constant cross-sectional area of the reactor, Ω. The transport takes place only along the length coordinate axis, x.

Possible reductions in lost work can give economic gains. The relation between reductions in lost work and economic gains is not unique, however, it varies for instance with energy prices. We consider it valuable to do energy optimization studies also separate from economic analyses.

Minimization of W_{lost} means minimization of the integral of σ, so we shall proceed with the integral only. We shall refer to minimization of the integral of σ as minimization of the lost work. The minimum value of the integral shall be called the minimum total entropy production rate. The minimization is carried out with the requirement of a constant production rate, J (in mol/h):

$$J = \Omega \int r dx \tag{2}$$

where r is the reaction rate. Minimization without this constraint gives the meaningless result of $\sigma = 0$. It is normal in engineering contexts to optimizate under constraints, and it is then common practice to use the Euler-Lagrange method [9], [2].

The question that we shall ask by the minimization procedure, is the following: Given J, how can we operate the reactor so that we obtain minimum lost work? The answer to the problem is an ideal answer in the way that it results in operating conditions or designs which may be unattainable. It is not the aim here to discuss in detail the practical construction or operation of the ideal reactor. We shall present a method that can be used to im-

prove actual operations. Minimum lost work can mean the highest possible temperature of the outlet cooling fluid, and in a subsequent article we shall demonstrate that this is so.

The present work can be seen as a continuation of our effort to find the reduce lost work in process equipments. The path of minimum lost work was obtained by us for distillation columns [5],[6], but has long been the target of optimization [?]. The study of chemical reactors in this context is newer,[7],[8],[10]. We have previously used a linear relation between the fluxes and the forces of transport in the cases we have studied. In this work we study situations where the rate, r, is not necessarily a linear function of the driving force (the reaction affinity or Gibbs energy of reaction). A short version of the article has been presented [3].

We shall use a plug flow reactor as our model case, as evident already from Eqs.(1) and (2). The results for batch reactors will be the same. In the batch reactor one integrates over time, while in the plug flow reactor, one integrates over space. The developments in time or space are in this respect equivalent, so we need only give equations for one type of reactor, see also [7].

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