

## Lyapunov based control for non isothermal continuous stirred tank reactor

H. Hoang\*F. Couenne\*C. Jallut\*Y. Le Gorrec\*

\*LAGEP, University of Lyon 1 - UMR CNRS 5007, Bât. 308 G  
 43, Bd du 11 nov. 1918, 69622 Villeurbanne cedex France,  
 name@lagep.univ-lyon1.fr

**Abstract:** In this contribution we apply the approach of passivity proposed by Ydstie [M. Ruzskowski, V. Garcia-Osorio, and B.E. Ydstie. *AIChE Journal*, 2005] for physico-chemical processes. The originality of this work lies in the fact we consider a thermodynamically nonlinear consistent model for a continuous stirred tank reactor to build the appropriate Lyapunov function for stabilization purpose. Indeed the kinetics of reaction modelled by Arrhenius law leads to non linear model with multiple steady state. We propose to stabilize the reactor around the unstable point. In order to apply the Ydstie approach, we assume that the fluid remains homogeneous. This assumption permits to use the concavity property of the entropy function to build the Lyapunov function. We propose feedback laws in order to ensure the closed loop properties of the Lyapunov function. Finally we propose some simulation results.

Keywords: Lyapunov based control, thermodynamics, Non isothermal CSTR.

### 1. INTRODUCTION

Control of Continuous Stirred Tank reactor (CSTR) has been widely investigated Luyben [1990], Read [1998], Alvarez [2000], Hua [2000], Guo [2001], Biagiola [2004], Jana [2005]. The underlying motivation relies on the fact that industrial chemical reactors may be operated at unstable operating conditions, which often corresponds to optimal process performance. The methodologies used for stabilization of such processes are often based on input/output (I/O) feedback linearization Bastin [1997] or nonlinear PI control algorithms Alvarez [1999, 2000]. In this paper we propose a Lyapunov based approach for the stabilization of CSTR around an unstable steady state. This approach is based on the recent work of Alonso [1997], Ydstie [1997], Ruzskowski [2005] where a thermodynamical development is given in order to obtain a Lyapunov function for transport reaction systems. In Ruzskowski [2005] the authors treat the example of CSTRs in the isothermal case.

### 2. THERMODYNAMIC ASPECTS

In this section we briefly review the basis of thermodynamics and show how to obtain the so called availability function. This availability function is a function issued from the second principle of the thermodynamic that is naturally positive for homogeneous thermodynamical systems. Consequently it is a natural candidate as Lyapunov function. We shall show this function issued from thermodynamic properties can be used for closed loop dynamic stabilization.

In Ruzskowski [2005] the authors apply fundament of irreversible thermodynamics in order to produce a Lyapunov function for stabilization purposes. Indeed thermodynamics is based on the concept of energy as well as Lyapunov functions. Moreover process systems are based for

their modelling on thermodynamics properties. In Ydstie [1997] the authors showed that passivity is related to the availability function used in thermodynamics for phase stability.

In the case of simple homogeneous thermodynamical systems composed of a mixture of  $n_c$  species, the fundamental relation of thermodynamics expresses the entropy  $S$  as a function of the internal energy  $U$ , the volume  $V$  and the mole number  $n_i$  by The Gibbs equation:

$$dS = \frac{1}{T}dU + \frac{P}{T}dV + \sum_{i=1}^{n_c} \frac{-\mu_i}{T}dn_i \quad (1)$$

where  $P$ ,  $T$ ,  $\mu_i$  represent respectively the pressure, the temperature and the chemical potential of species  $i$ . It is well known that balance equation can be established for  $U, V$  and  $n_i$  as well as for the entropy  $S$  but this latter is not conservative. let us consider the vector of extensivities  $Z^T = (U \ V \ n_1 \ \dots \ n_c)$  and its associated vector of intensities (homogeneous function of degree 0 of

$$Z) \ w^T = \left( \frac{1}{T} \ \frac{P}{T} \ \frac{-\mu_1}{T} \ \dots \ \frac{-\mu_c}{T} \right). \text{ It then follows that}$$

$$w = \frac{\partial S}{\partial Z}. \quad (2)$$

*Remark 1.* Gibbs equation (1) differentiation with respect to time permits to link together the different balance by:

$$\frac{dS}{dt} = w^T \frac{dZ}{dt}. \quad (3)$$

$S$  being a homogeneous function of degree 1 with respect to  $Z$ , from Euler's theorem we can express entropy as:

$$S = w^T Z. \quad (4)$$

In the case of isolated systems, the entropy balance is reduced to:

$$\frac{dS}{dt} = \sigma. \quad (5)$$

where the entropy production term  $\sigma$  is positive from the second law of thermodynamics. The entropy  $S$  of an isolated system can only increase. In this case the irreversibilities will be due to non equilibrium initial conditions over the considered domain. As a consequence for simple homogeneous thermodynamical systems, the entropy function  $S(z)$  is necessarily concave (see Callen [1985]) as shown in figure 1.

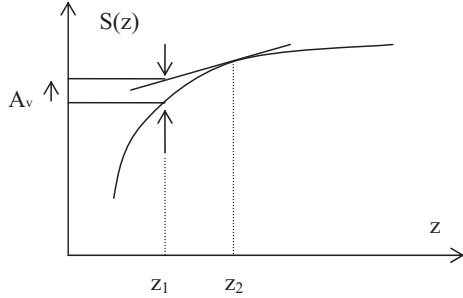


Fig. 1. Entropy function with respect to  $Z$  and the availability

From these observations, it can be shown (see Ydstie [1997]) that the non negative function  $A_v(Z_1) = S(Z_2) + w_2^T(Z_1 - Z_2) - S(Z_1)$  is a measure of the distance between the state  $Z_1$  and the thermodynamic  $Z_2$ . The slope of the tangent plane is related to intensive vector.

*Remark 2.* The availability  $A_v$  corresponds to the quantity involved in the Gibbs' tangent plane condition: Gibbs (1873) proved that any given mixture at a given temperature pressure and overall composition would be globally stable if and only if the tangent to the Gibbs free energy surface (not necessarily concave) would never cut the surface. This result is used effectively to solve the multiphase equilibrium problems. In the case of entropy surface it means that  $A_v$  must be non negative.

In more general case, we get that two states  $Z$  and  $Z_2$  are in equilibrium if and only if  $A_v(Z) = Z_2 = 0$ .

So as soon as we consider homogeneous mixture,  $S$  remains concave and  $A$  can be considered as a Lyapunov function candidate. It remains to set feedback control such that

$$\frac{dA_v}{dt} < 0. \quad (6)$$

### 3. DESCRIPTION OF THE CSTR MODEL

In the present paper we consider a CSTR that is connected to a heat exchanger that is used to control the temperature within the reactor. The dynamics of the stirred tank reactor (STR) can be deduced from mass and energy balances by considering the following assumptions:

- The heat flow exchanged with the jacket is represented by  $Q$  ( $w$ ) and depends on the temperatures of the jacket  $T_w$  and of the reactional mixture in the reactor  $T$ :  $Q = \lambda(T_w - T)$  with  $\lambda$  the heat transfer coefficient ( $w/K$ ).

- The reaction under consideration  $A \rightarrow B$  takes place in the reactor in liquid phase. The kinetics of the reaction is modelled by the Arrhenius law. The reaction rate  $r_v$  is given by  $k_0 \exp \frac{-E}{RT} \frac{n_A}{V}$ .
- the reaction mixture is supposed to be ideal.
- For simplicity, the two species are supposed to have the same molar volume  $v_A = v_B = v$  ( $m^3/mol$ ).
- At the inlet of the reactor, the pure component  $A$  is injected at temperature  $T_e$ .
- the reaction volume  $V$  is supposed to be constant as well as the pressure  $P$ . This implies a constraint on the total outlet flow. Moreover  $P$  is set to  $P_{ref}$ .

#### 3.1 CSTR modelling

The mass balance are given by:

$$\begin{cases} \frac{dn_A}{dt} = F_{Ae} - F_A - \xi_A r_v V \\ \frac{dn_B}{dt} = -F_B + \xi_B r_v V \end{cases} \quad (7)$$

where

- $n_A, n_B$  are the mole number of species  $A$  and  $B$  respectively ( $mol$ ).
- $F_{Ae}$  is the inlet molar flow rate of species  $A$  ( $mol/s$ ).
- $F_A, F_B$  are the outlet molar flow rate of species  $A$  and  $B$  respectively ( $mol/s$ ).
- $\xi_A, \xi_B$  are the stoichiometric coefficient (supposed to be equal to 1).

let us write the internal energy balance:

$$\frac{dU}{dt} = Q - P \frac{dV}{dt} + F_{Ae} h_{Ae} - \overbrace{F_A h_A - F_B h_B}^{\text{flowing out enthalpy}}, \quad (8)$$

where

- $U$  is the internal energy ( $J$ ).
- $h_{Ae}$  is the inlet molar enthalpy of species  $A$  ( $J/mol$ ).
- $h_i$  is the molar enthalpy of species  $i$  ( $i = A, B$ ) in the reactor ( $J/mol$ ).
- $P$  is the pressure in the reactor ( $Pa$ ).

*Remark 3.* Since we suppose ideality of the mixture, the enthalpy of species in the mixture can be expressed as:  $h_A(T) = c_{pA}(T - T_{ref}) + h_{Aref}$  A same expression can be written for  $B$ . where  $c_{pA}$  ( $J/mol/K$ ) is the heat capacities of species  $A$ ,  $T_{ref}$  is the reference temperature,  $h_{Aref}$  is the enthalpy of reference of species. Let us note furthermore that, as the species are involved in a chemical reaction, the reference molar enthalpies have to be chosen with regard to the enthalpy of formation of species.

Finally the volume balance is given by:

$$\frac{dV}{dt} = 0 \quad (9)$$

Moreover the volume is also given by:  $V = \sum_{i=A,B} n_i v_i$ . Deriving this expression and equating to zero, the total output flow rate  $F$  is deduced. Since  $F_A = x_A F$  and  $F_B = x_B F$  where  $x_A$  and  $x_B$  represent the mole fraction of species  $A$  and  $B$  respectively, we get:

$$F = \frac{v_A F_{Ae} + (\xi_B v_B - \xi_A v_A) r_v V}{x_A v_A + x_B v_B} \quad (10)$$

*Remark 4.* let us note that  $x_A = \frac{n_{AV}}{V}$

### 3.2 Analysis of the steady states

A most interesting feature of this reactor that creates control difficulty is its multiple steady states. Figure 1 illustrates this feature clearly. There are three steady state operating points:  $P_1$ ,  $P_2$  and  $P_3$ . The steady state operating points  $P_1$  and  $P_3$  are stable, whereas the steady state operating point  $P_2$  is not stable. The reactor is operated at unstable steady state operating point  $P_2$  which is at medium conversion. Manipulated variables are chosen as:

$$F_{Ae} = 0.0183 \frac{\text{mole}}{\text{s}}, T_e = 310 \text{ K and } T_w = 300 \text{ K} \quad (11)$$

The steady state points are computed using equations 7 and 8 considering  $\frac{dn_a}{dt} = \frac{dn_b}{dt} = \frac{U}{dt} = 0$  and the relation between  $U$  and  $T$ . The steady states operating points are:

$$[n_A \ n_B \ T] = [1.6449 \ 0.3551 \ 320.6704] \text{ (P1)}$$

$$[n_A \ n_B \ T] = [1.3583 \ 0.6417 \ 330.1997] \text{ (P2)}$$

$$[n_A \ n_B \ T] = [0.1416 \ 1.8584 \ 377.8795] \text{ (P3)}$$

as shown in figure 2, where  $F$  corresponds to the right member of the differential equation written with respect to temperature  $T$ :

$$F = (h_A - h_B) r_v V + F_{Ae} C_{pA} (T_e - T) + \lambda (T_w - T).$$

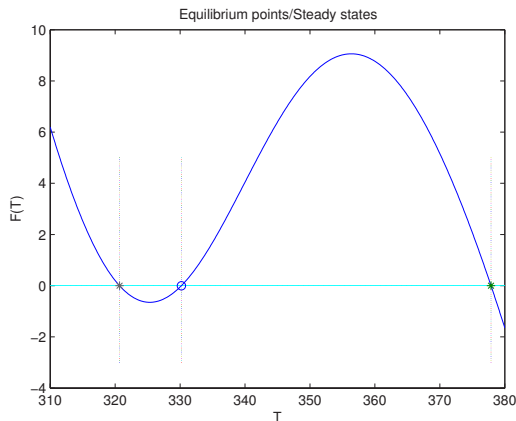


Fig. 2. Steady states reactor temperature vs.  $F(T)$

### 3.3 Controller synthesis

The control objective of this system is to maintain the reactor temperature  $T$  as well as mole number  $n_B$  at their desired value by manipulating the coolant temperature  $T_w$ , the inlet molar flow rate of species  $A$   $F_{Ae}$  as well as its temperature  $T_e$ .  $T_e$  appears in the inlet enthalpy of species  $A$   $h_{Ae}$ .

The availability function has to be written with  $w = \left(\frac{1}{T}, \frac{P}{T}, -\frac{\mu_A}{T}, -\frac{\mu_B}{T}\right)$  et  $Z = (U, V, n_A, n_B)$ . Nevertheless since the reactional scheme is very simple with constant volume and same molar volume for species, we have the constraint between  $n_A$  and  $n_B$ :

$$-\frac{dn_A}{dt} = \frac{dn_B}{dt} \quad (12)$$

and with (9), we can rewrite  $A$  with  $w = \left(\frac{1}{T}, -\frac{\mu_A}{T} + \frac{\mu_B}{T}\right)$  et  $Z = (U, n_A)$ .

Let us rewrite the availability function of this process with respect to  $P_2$ :  $A(Z) = S_2 + w_2^T (Z - Z_2) - S(Z)$ . From equation (4), we obtain:

$$\frac{dA_v}{dt} = -(w - w_2)^T \frac{dZ}{dt} \quad (13)$$

Considering the deviation variable  $\tilde{w} = w - w_2$ , (13) can be expressed by:

$$\frac{dA_v}{dt} = -\tilde{w}^T \frac{dZ}{dt} \quad (14)$$

$$\frac{dA_v}{dt} = -\tilde{w}^T \begin{pmatrix} Q + F_{Ae} h_{Ae} - F_A h_A - F_B h_B \\ F_{Ae} - F_A - r_v V \end{pmatrix} \quad (15)$$

With simplifying assumptions<sup>1</sup> molar volume and stoichiometric coefficient the total molar flow rate becomes:

$$F = v F_{Ae} \quad (16)$$

and we get

$$\frac{dA_v}{dt} = -\tilde{w}^T \begin{pmatrix} Q(T_w) + \mathfrak{F}(T_e) F_{Ae} \\ \mathfrak{G} F_{Ae} - r_v V \end{pmatrix} \quad (17)$$

with  $\mathfrak{F} = h_{Ae}(T_e) - v(x_A h_A(T) + (1 - x_A) h_B(T))$ ,  
 $\mathfrak{G} = 1 - v x_A$

The objective is to set feedback control on the manipulated variables  $T_w$ ,  $T_e$  and  $F_{Ae}$  such that  $\frac{dA_v}{dt} < 0$ . It is done expressing  $\frac{dA_v}{dt}$  as a semi definite negative quadratic form respect to the variables  $\tilde{w}$ . Let us choose:

$$Q = -K_1 \left( \frac{1}{T} - \frac{1}{T_2} \right). \quad (18)$$

From this equation, the manipulated temperature feedback law  $T_w$  is deduced as:

$$T_w = \frac{K_1}{\lambda} \left( \frac{1}{T} - \frac{1}{T_2} \right) + T \quad (19)$$

$T_e$  is chosen such that  $\mathfrak{F} = \mathfrak{F}(T_e, T, n_A, n_B) = 0$ . Finally  $F_{Ae}$  is chosen such that:

$$F_{Ae} = \mathfrak{G}^{-1} \left( r_v V + K_2 \left( \widetilde{-\frac{\mu_A}{T} + \frac{\mu_B}{T}} \right) \right) \quad (20)$$

Where

$$\left( \widetilde{-\frac{\mu_A}{T} + \frac{\mu_B}{T}} \right) = \left( -\frac{\mu_A}{T} + \frac{\mu_B}{T} \right) - \left( -\frac{\mu_{A2}}{T_2} + \frac{\mu_{B2}}{T_2} \right)$$

We then obtain:

$$\frac{dA_v}{dt} = -\tilde{w}^T \mathfrak{K} \tilde{w} \quad (21)$$

<sup>1</sup> Even if they simplify the notation, these assumptions are not necessary for the design of the control law.

with  $\hat{\mathfrak{K}} = \begin{pmatrix} K_1 & 0 \\ 0 & K_2 \end{pmatrix}$ .

Since the  $K_i$ 's are chosen strictly positive clearly  $\frac{dA_v}{dt} < 0$  so  $A_v$  tends exponentially to zero.

### 3.4 Simulation

The purpose of this section is to illustrate the stabilization procedure on a simple but realistic example. Parameters used for simulation are given in table 1 and simulations are carried out using Matlab Simulink software.

	Numerical value
$C_{pA}$	75.24
$C_{pB}$	60.
$E$	1046.43
$h_{Aref}$	0
$h_{Bref}$	-4575
$k_0$	$0.12 \cdot 10^{10}$
$P$	$10^5$
$P_{ref}$	$10^5$
$R$	$8.314(J/K/mol)$
$T_{ref}$	300
$v$	0.0005
$V$	0.001
$\lambda$	0.05808
$s_{Aref}$	210.4
$s_{Bref}$	180.2
$\xi_A$	1
$\xi_B$	1

Table 1. Steady-state design parameters

First of all let us consider open loop simulation with input (11) and initial state P2. As operating point P2 is the most interesting from industrial point of view we do simulations around this point. Let us note that P2 corresponds to a good advancement of the reaction and to a moderate temperature which is usually necessary to preserved good quality of polymers for example. This steady state is typically unstable. From any point of the operating domain the system can go to the stable steady state P1 where the reaction is shutting down (low temperature) or to the stable steady state P3 if the reaction go faster (high temperature). The operating point P2 is very sensitive to small variations or errors on the initialization. Indeed despite high accuracy in the steady state computation (say precision around  $10^{-5}$ ) the system accumulate numerical errors and tends after a certain time to the nearest steady state point P1 (see Figure 3).

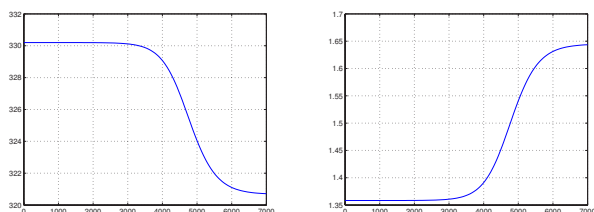


Fig. 3. Open loop simulations around the unstable steady state. Reactor temperature (lhs) and number of moles of species A (rhs) vs. time)

It can be shown that this steady state is also sensitive to input and initial state perturbations. In a second step we implement the proposed feedback strategy (19,20) with  $K_1 = 500, K_2 = 10$  and proceed to the same simulation around the operating point P2 (see figure 4)

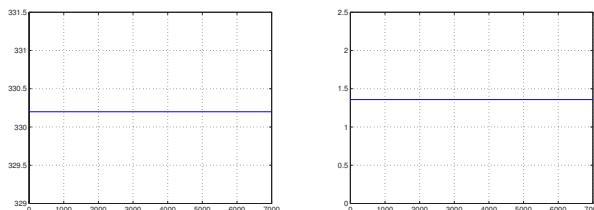


Fig. 4. Closed loop simulations around the unstable steady state. Reactor temperature (lhs) and number of moles of species A (rhs) vs. time)

One can notice that temperature and composition stay at there initial values. The Lyapunov function plays its role and insures that numerical errors around this equilibrium point decrease respect to time. Even if simulation are carried on over larger time domain the steady state remains stable. To emphasis this phenomenon we proceed to the same simulation with error on the initial state (initial temperature is set equal to 304 K) (figure 5).

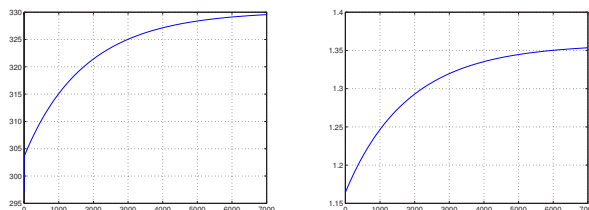


Fig. 5. Closed loop simulations around the unstable steady state with different initial state. Reactor temperature (lhs) and number of moles of species A (rhs) vs. time)

Again the Lyapunov function insures the system remains stable around the operating point P2. The temperature and the composition of the mixture join more or less faster the values corresponding to the desired steady state. Let us note that the dynamic behavior of the error depends on the values of the parameters  $K_1$  and  $K_2$ .

The results presented here are quite satisfactory from a qualitative point of view. We shown that thermodynamic naturally proposes Lyapunov function usable for dynamic control. Nevertheless it is only a first step for the realistic control of non isothermal continuous reactors as one have to take care of input sollicitation, state variable observation and closed loop performances. Similar thermodynamic concepts could be applied on the global system including the observer in order to insure the global stability of the closed loop system.

## 4. CONCLUSION

The present work provides a Lyapunov based control for a nonisothermal CSTR. The control objective in this

simulation-based work is to maintain the CSTR at steady state operating point. The main difficulty arises when the operating point is unstable. This study is a first attempt to build a Lyapunov function for thermodynamical coherent CSTR from Ydstie's work (Ydstie [1997], Alonso [1997], Ruszkowski [2005]). Clearly the control feedback must be improved: two manipulated variables must be used instead of three. Moreover this controller must be coupled with an observer since all the state variables are used.

#### REFERENCES

- B.E. Ydstie, and A.A. Alonso. Process systems and passivity via the Clausius-Planck inequality. *Systems Control Letters*, 30(5):253-264, 1997.
- A.A. Alonso, and B.E. Ydstie. Process systems, passivity and the second law of thermodynamics. *Computers and Chemical Engineering*, 20(2):1119-1124, 1996.
- M. Ruszkowski, V. Garcia-Osorio, and B.E. Ydstie. Passivity based control of transport reaction systems. *AIChE Journal*, 51:3147-3166, 2005.
- B. Guo, A. Jiang, X. Hua, X., and A. Jutan. Nonlinear adaptive control for multivariable chemical processes. *Chemical Engineering Science*, 56:6781-6791, 2001.
- M.A. Henson. Nonlinear Model Predictive Control: Current Status and Future Directions. *Computers and Chemical Engineering*, 23:187-202, 1998.
- X. Hua, and A. Jutan. Nonlinear Inferential Cascade Control of Exothermic Fixed-bed Reactors. *AIChE Journal*, 46:980-996, 2000.
- A.K. Jana, A.N. Samanta, and S. Ganguly. Globally linearized control on diabatic continuous stirred tank reactor: a case study. *ISA Transactions*, 44:423-444, 2005.
- K.J. Kim, and K.Y. Choi. On-line estimation and control of a continuous stirred tank polymerization reactor. *Journal Process Control*, 1:96-110, 1991.
- C. Kravaris, and C.B. Chung. Nonlinear state feedback synthesis by global input/output linearization. *AIChE Journal*, 33:592-603, 1987.
- P.L. Lee, and G.R. Sullivan. Generic Model Control (GMC). *Computers and Chemical Engineering*, 12:573-580, 1988.
- W.L. Luyben. *Process Modeling, Simulation, and Control for Chemical Engineers*. McGraw-Hill, Singapore, 1990.
- L. Magni, G. De Nicolao, L. Magnani, and R. Scattolini. A stabilizing model-based predictive control algorithm for nonlinear systems. *Automatica*, 37:1351-1362, 2001.
- N.K. Read, and W.H. Ray. Application of nonlinear dynamic analysis to the identification and control of nonlinear systems III. n-Dimensional systems. *Journal of Process Control*, 8(1):35-46, 1998.
- J. Alvarez-Ramirez, and A. Morales. PI control of continuously stirred tank reactors: stability and performance. *Chemical Engineering Science*, 55(22):5497-5507, 2000.
- C.T. Chen, and C.S. Dai. Robust controller design for a class of nonlinear uncertain chemical processes. *Journal of Process Control*, 11(5):469-482, 2001.
- S.I. Biagiola, and J.L. Figueroa. A high gain nonlinear observer: application to the control of an unstable nonlinear process. *Computers and Chemical Engineering*, 28(9):1881-1898, 2004.
- F. Viel, and F. Jadot, and G. Bastin. Global stabilization of exothermic chemical reactors under input constraints *Automatica*, 33(8):1437-1448, 1997.
- J. Alvarez-Ramirez, and R. Femat. Robust PI stabilization of a class of chemical reactors. *Systems & Control Letters*, 38(4-5):219-225, 1999.
- H.B. Callen. *Thermodynamics and an introduction to thermostatics*. JohnWiley & Sons Inc, 2nd ed. New York, 1985.