# MODEL PREDICTIVE CONTROL OF A CATALYTIC FLOW REVERSAL REACTOR WITH HEAT EXTRACTION

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Abstract:
This paper presents the formulation of a controller for a Catalytic Flow Reversal Reactor (CFRR) with heat extraction. The controller is based on the Model Predictive Control (MPC) concept. The MPC scheme uses a model that assumes plug flow and neglects radial gradients in the reactor but accounts for the two phases within the reactor. The prediction of the future output behavior from the model is obtained by using the Method of Characteristics as proposed by Shang *et al.* (2004) for convection dominated distributed parameter systems. The formulated controller is applied to a CFRR unit for the catalytic oxidation of fugitive lean methane mixtures. The objective of the control algorithm is to maintain stable reactor operation, while extracting the maximum amount of useful energy by hot gas removal from the mid-section of the reactor. Simulations are used to show the performance of the designed controller.

Keywords: Reverse Flow Reactor, Model Predictive Control, Method of Characteristics.

## 1. INTRODUCTION

Catalytic Flow Reversal Reactor (CFRR) technology has received much attention in recent years (Matros and Bumimovich, 1996) and has been proposed for many applications including: methane combustion, oxidation of volatile organic compounds (VOC), oxidation of sulphur dioxide (SO2) and the synthesis of methanol.

CFRR has recently been suggested for the combustion of lean methane streams (Hayes, 2004). Fugitive lean methane streams are common in the oil and gas industry and are a great source of pollutant emission. Sources of methane emissions include leaks in natural gas transmission facilities such as pipelines and compression stations and upstream oil and gas production facilities, especially from solution gas. These methane emissions are typically available at ambient temperatures, where catalytic reaction rate is very slow, but the use of reverse flow technology has been shown to be feasible technology to achieve sufficiently high reactor temperatures (Hayes, 2004).

The primary advantage of the technology is that the thermal capacity of the solid material within the reactor acts as a regenerative heat exchanger, allowing authothermal operation without the use of heat exchangers. For exothermic reactions, switching the flow direction periodically creates a heat trap effect. This effect can be used to achieve and maintain an enhanced reactor temperature

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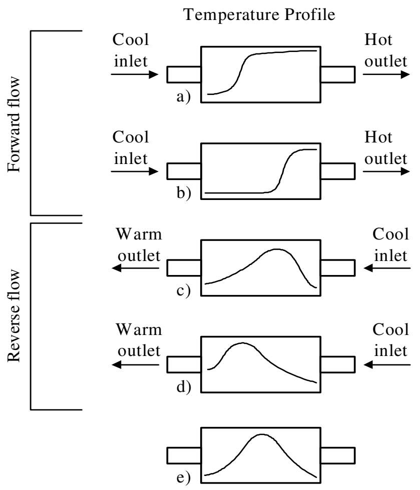


Fig. 1. Illustration of the heat trap effect for reverse flow operation.

compared to a single flow direction mode of operation.

The principle of the heat trap effect is illustrated in Figure 1. Figure 1(a) illustrates a reactor temperature profile that might be observed in a standard uni-directional flow operation for a combustion. If a temperature pattern, shown in Figure 1(a) and (b) is established, the reverse flow operation can then be used to take advantage of the high temperatures near the reactor exit to pre-heat the reactor feed. A quasi-steady state operation may be achieved in which the reactor temperature profile has a maximum value near the centre of the reactor, which slowly oscillates as the feed is switched between the two ends of the reactor, as shown in Figure 1(c-e).

The control of the CFRR is a particularly challenging problem. In addition to the complexities of any distributed parameter tubular reactor (i.e. nonlinear distributed dynamics and limited on-line measurement information), the CFRR presents periodic change of feed flow direction.

When controlling the CFRR, the main objective is to maintain the reactor operating in a region where the temperature in the active sections (catalyst sections) is below a critical value to avoid overheating or deactivation of catalyst and is above the extinction temperature of the reaction. The CFRR system is open-loop is stable. However, disturbances (i.e. inlet concentration), if sufficiently large, can extinguish the reaction or burn the catalyst. Different designs and control measures have been proposed to control the CFRR (Nieken *et al.*, 1994) including: bypassing the flow in the mid-section of the reactor, withdrawing of gas to a external cooler and cooling of the entire mid-section by using a heat exchanger.

The first work on feedback control for the CFRR was done by Budman *et al.* (1996). Two control strategies for a CO oxidation unit were discussed in their work: a PID feedback loop used to control the outlet concentration by manipulation of the cooling rate in the mid-section of the reactor and a feed-forward scheme that measures inlet concentration and select optimal cycle period and cooling rate from a parametric map. Barresi and Vanni (2002) discuss the use of a feedback logic controller, with cycle period as manipulated variable, to avoid extinction of the reaction in a volatile organic compounds (VOC) CFRR unit. More recently, a Model Predictive Control (MPC) was proposed to control a VOC combustor with flow reversal operation (Dufour and Couenne, 2003; Dufour and Toure, 2004) by using a power supply at the core of the reactor and inlet dilution. In the MPC formulation, a linear model obtained from the linearization of a nonlinear distributed parameter system model about a fixed operating point was used.

The aim of this paper is to present a control scheme that can be used to maintain the CFRR at a stable operational conditions, while extracting the maximum amount of hot gas from the reactor.

We investigate the use of heat removal by mass extraction from the middle section of the reactor as a manipulated variable. Extraction of a hot stream has an additional benefit of providing energy that can be used for many purposes such as heating and power generation (Kushwaha *et al.*, 2005). Hot gas withdrawal has been proposed in the literature to avoid overheating of the CFRR unit, but none of the control strategies published in the literature for the CFRR use the gas withdrawal from the mid-section as a control variable.

With this work, we contribute with the application of a Model predictive Control to a distributed parameter flow system with periodic oscillation of the flow direction. The controller is designed using the MPC scheme proposed by Shang *et al.* (2004) for convection-dominated distributed parameter systems where the Method of Characteristics (Arnold, 1988) is used to predict future output behaviour of the controlled plant. By applying this scheme to a CFRR unit we are extending its application to a distributed parameter system with output constraints. The method of characteristics for convection dominated systems (hyperbolic partial differential equation models) is simple and systematic and provides a geometric way of viewing the solution structure and can help in providing insight into the future evolution of the process output.

The work presented here is focused on the development of a candidate MPC scheme that will produce a high level of performance for the CFRR and to investigate the computational challenges inherent in this problem.

## 2. CONTROL SYSTEM DESIGN

In this work, a model of the CFRR unit to be controlled is used to predict the future behavior of the plant. The performance of the plant is optimized over a future finite horizon according to the current state of the plant. A sequence of manipulated variable adjustments is determined by optimizing an open-loop performance objective on a time interval extending from the current time through a specified prediction horizon. The computed settings for the manipulated variables are implemented and kept constant until the next control interval. Feedback is incorporated by using the measurements to correct modeling errors and update the disturbance estimate in the optimization problem for the next time step.

### *2.1 Modelling*

The reactor consists of two parallel sections with an internal diameter of 0.2 metres mounted side by side and connected by a U-bend at the bottom (total length = 2.73 m). The reactor internals consist of a combination of open spaces, inert (monolith) sections and active catalyst (packed-bed) sections, as shown in Figure 2. A heterogeneous one-dimensional model is used to predict the future output behavior of the CFRR. The model is a simplified version of the two-dimensional heterogeneous model developed by Salomons *et al.* (2004). The basic equations for the mass and energy balance in the CFRR reactor, assuming plug flow, are:

$$\frac{\partial(Y_f)}{\partial t} + \alpha v_s \frac{\partial(Y_f)}{\partial x} = k_m a_v (Y_s - Y_f) \quad (1)$$

$$\frac{\partial(T_f)}{\partial t} + \alpha v_s \frac{\partial(T_f)}{\partial x} = \frac{h a_v}{\rho_f C p_f}(T_s - T_f) \quad (2)$$

$$k_m a_v C_f (Y_f - Y_s) = (1-\epsilon)\eta k_R C_s \quad (3)$$

$$\frac{\partial(T_s)}{\partial t} = \frac{\eta k_R C_s Y_s (-\Delta H_R)}{\rho_s C p_s} + h(T_f - T_s) \quad (4)$$

with boundary conditions $Y_f(t,0) = Y_{f_0}$ and $T_f(t,0) = T_{f_0}$, where $Y_f$ and $T_f$ are the mole fraction of methane and temperature of the fluid phase, $Y_s$ and $T_f$ are their counterpart in the solid phase, $(1-\alpha)$ is the fraction of mass extracted and $v_s$ is the superficial velocity of the gas stream. Values for the various parameters in the model are given in Salomons *et al.* (2004).

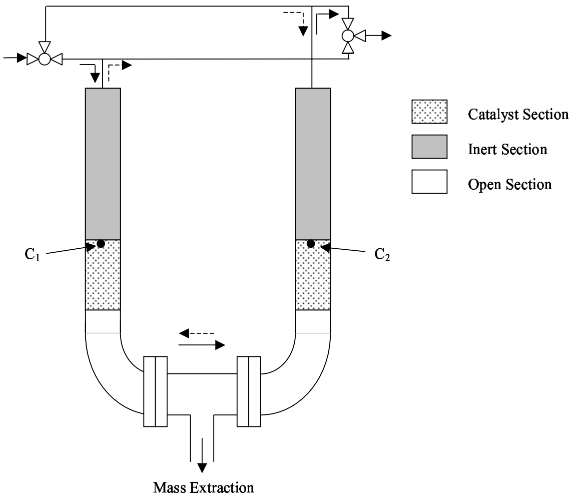


Fig. 2. Schematic picture of the CFRR reactor.

The dynamic behaviour of the CFRR is dominated by the energy balance in the solid phase, equation 4, while the dynamics of the mole and energy balance in the fluid phase are fast owing to the short residence time of the fluid in the reactor and the low thermal mass of the fluid. The resulting system of equations (1)-(4) can be solved using the method of characteristics (Acrivos, 1956). Equations (1) and (2) can be described by a system of ODEs along the characteristic curve $\xi_1$:

$$\xi_1 = \frac{dx}{dt} = \alpha v_s \quad (5)$$

Along $\xi_1$, the state variables $Y_f$ and $T_f$ are described by:

$$\frac{dY_f}{dt} = k_m a_v (Y_s - Y_f) \quad (6)$$

$$\frac{dT_f}{dt} = \frac{h a_v}{\rho_f C p_f}(T_s - T_f) \quad (7)$$

On the other hand, the energy balance equation in the solid phase varies along the time axis only, and its solution is described along a constant second characteristic line, $\xi_2$, by:

$$\frac{dT_s}{dt} = \frac{\eta k_R C_s Y_s (-\Delta H_R)}{\rho_s C p_s} + h(T_f - T_s) \quad (8)$$

The future output is predicted by numerically integrating the system of equations:

$$\frac{dx}{dt} = \alpha v_s \quad (9)$$

$$\frac{dt}{dt} = 1 \quad (10)$$

$$\frac{dY_f}{dt} = k_m a_v (Y_s - Y_f) \quad (11)$$

$$\frac{dT_f}{dt} = \frac{h a_v}{\rho_f C p_f}(T_s - T_f) \quad (12)$$

$$\frac{dT_s}{dt} = \frac{\eta k_R C_s Y_s (-\Delta H_R)}{\rho_s C p_s} + h(T_f - T_s) \quad (13)$$

$$k_m a_v C_f (Y_f - Y_s) = (1-\epsilon)\eta k_R C_s \quad (14)$$

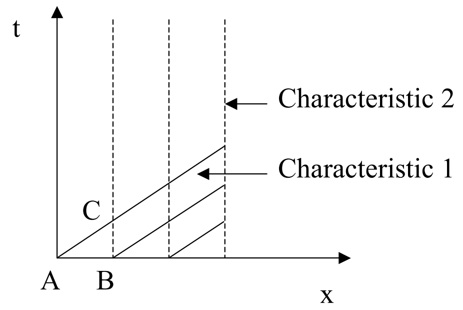


Fig. 3. Schematic picture of the CFRR reactor.

Predictions of future output values are obtained by discretizing the initial state at a finite number of spatial points, projecting the characteristic curves from each of these points and then computing the values of the state variables at the intersection points. Figure 3 illustrates the calculation of the state variables at point C from the values at points A and B. The segment AB is the domain of dependence of point C, given that the values of state variables at point C are completely defined by the state-variable values on the segment AB. By varying point C and repeating the procedure, the values of the state variables at different grid points and different future times can be calculated. The value of the state variables at the intersection points is obtained by integrating the differential equations using, for example, the Euler or mplicit Euler method and solving the resulting system of nonlinear equations. Using the output prediction method described above, the value of the output for a prediction horizon time is obtained for specific control actions. To use the predictions in the MPC scheme, the predicted output is expressed in a locally linear form (Shang *et al.*, 2004):

$$\hat{\mathbf{y}} = \hat{\mathbf{y}}_{\mathbf{0}} + \mathbf{S}\boldsymbol{\Delta}\mathbf{u} \tag{15}$$

$$\hat{\mathbf{y}}_{\mathbf{0}} = \mathbf{y}_0 + \mathbf{S}[u_{-1}, u_{-1}, \cdots, u_{-1}]^T \tag{16}$$

$$\boldsymbol{\Delta}\mathbf{u} = [u_0 - u_{-1}, \cdots, u_{H_c-1} - u_{-1}]^T \tag{17}$$

where $\hat{\mathbf{y}}_{\mathbf{0}}$ is the vector of predicted outputs due to past control actions in the prediction horizon time, $\mathbf{y_0}$ is the vector of initial values of the state variable, $\boldsymbol{\Delta}\mathbf{u}$ is the vector of future control increments ($u \triangleq \alpha$; $\Delta u_i = \alpha_i - \alpha_{-1}$ $for$ $i = 0 \cdots H_C - 1$), $\hat{\mathbf{y}}$ is the vector of the predicted outputs and $\mathbf{S}$ is the rate of output variation about past control actions ($\mathbf{u}_{-1}$). The elements of $\mathbf{S}$ are updated at each sampling time and are computed via perturbation:

$$\mathbf{S} = \left(\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{u}}\right)_0 = \frac{\hat{\mathbf{y}}|_{\mathbf{u}_{-1+\delta}} - \hat{\mathbf{y}}|_{\mathbf{u}_{-1}}}{\delta} \tag{18}$$

where $\delta$ is a numerical perturbation on past input $\mathbf{u}_{-1}$, $\hat{\mathbf{y}}|_{\mathbf{u}_{-1+\delta}}$ and $\hat{\mathbf{y}}|_{\mathbf{u}_{-1}}$ are the predicted future output under the control actions $\mathbf{u}_{-1+\delta}$ and $\mathbf{u}_{-1}$. The future output is predicted up to an appropriate prediction horizon ($H_P$).

### *2.2 Optimization: Control Objective and Constraints*

The control objective is to maintain the reactor temperatures within an appropriate range so that overheating and/or reaction extinction are not possible. In this work we focus the attention on the extinction phenomena. This control objective is met by manipulating the flow of hot gas from the mid-section of the reactor. An additional control objective involves the extraction of the maximum amount of energy from the reactor. To achieve the control objective, the following finite horizon problem is solved at each sampling time ($k$):

$$\begin{aligned} &\min_{u(k+i|k)} \; J(u(k+i|k)) \\ &= \sum_{i}^{H_C-1} \left[\frac{\Delta u(k+i|k) - (u_{-1} + u_{min})}{(u_{max} - u_{min})}\right]^2 \end{aligned} \tag{19}$$

such that

$$u_{min} \leq u \leq u_{max}$$
$$\Delta u_{min} \leq \Delta u \leq \Delta u_{max}$$
$$T_{min} \leq T_s \leq T_{max}$$

The constraints are arranged in a linear vector inequality form and are softened by penalizing the $\infty$-norm of the constraint violations. Feedback is incorporated by comparing the actual measurement of the plant and the predicted output from the model. The resulting constrained quadratic optimization is solved using the active set method.

## 3. SIMULATIONS

To evaluate the performance of the designed controller, simulations of the CFRR unit and controller were implemented in the Matlab® environment. For all the simulation cases, an initial temperature profile, Figure 4, a set of boundary conditions $Y_f(t, x = 0) = 0.5$ $mol$ % $T_f(t, x = 0) = 298K$ and inlet flow velocity ($v_s(t, x = 0) = 0.2 \cdot m/sec$) are chosen. A fixed time for the flow reversal is chosen and setted to 300 sec. For the controller, the following parameters are used: $T_{sampling} = 50(sec)$, $H_P = 18T_{sampling} = 900(sec)$, $H_C = 1$, $0.6 \leq \alpha \leq 1$ and $|\Delta\alpha| = 0.05$.

The controller is then used to control the minimum temperature in the active catalyst sections (to avoid extinction of the reaction) while extracting the maximum amount of heat from the mid-section of the reactor. The minimum temperature can be chosen as the minimum temperature required to avoid extinction of the reaction or as the temperature that will give a high conversion

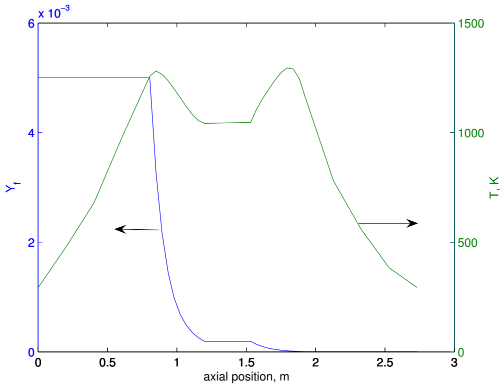


Fig. 4. Initial temperature ($T_f(0, x) = T_s(0, x)$ and concentration distribution along the axial distance of the reactor.

of reactants. If the latter is not known, then a constraint on the maximum allowable mol fraction of methane ($Y_f$) on the exit of each catalyst section can be added. In this work, a minimum temperature of 950 K is arbitrarily chosen for simulation purposes. The infinite dimensional process variables at the current time are discretized into $m = 60$ points along the axial direction of the reactor. It is assumed that all process variables can be measured at these discrete points.

The control performance is first evaluated with a simulated plant that matches exactly the the model used to predict the future output behavior of the CFRR unit (i.e. equations (1) - (4)). Figure 5(a)-(b) shows the output behaviour of the temperature at two points (marked as $C_1$ and $C_2$ in Figure 2). The temperature at the inlet of the catalytic sections are of great importance since most of the reaction takes place near the entrance to these sections. It can be seen from Figure 5(a)-(b) that the controller is able to drive the output to a new stationary state where the minimum temperature is above the desired temperature. Figure 6 shows the optimal fraction of total mass flow of hot gas that is extracted to achieve the desired control performance.

The control performance is also evaluated with a plant simulated with a highly detailed model . The new plant consist of a 2-dimensional heterogeneous model developed by Salomons *et al.* (2004) that is solved using the finite element method in Femlab®. The main structural difference of simplified 1-D model and the full 2-D model is the effect of the thermal insulation (thickness of insulation = 0.28 metres), which has been shown to be important for small diameter reactors and low air velocity conditions (Aube and Sapoundjiev, 2000; Salomons *et al.*, 2004). Figure 7(a)-(b) shows the output behavior of the temperature at the two points marked in Figure 2. It can be seen from Figure 7(a)-(b) that the controller is able to drive the output to a new stationary

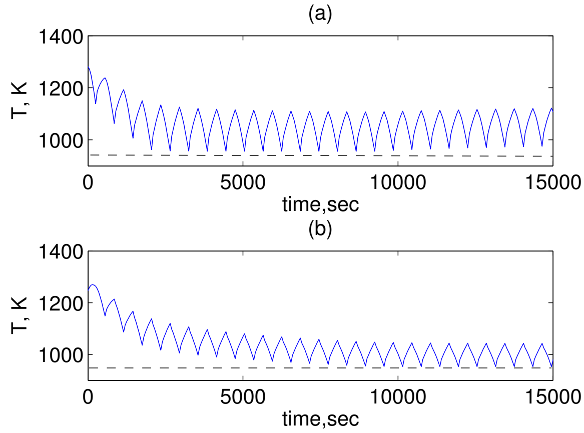


Fig. 5. (a) Temperature at point $C_1$ (see Figure 2) with control. (b) Temperature at point $C_2$ (see Figure 2) with control. The dashed line indicates the temperature lower bound.

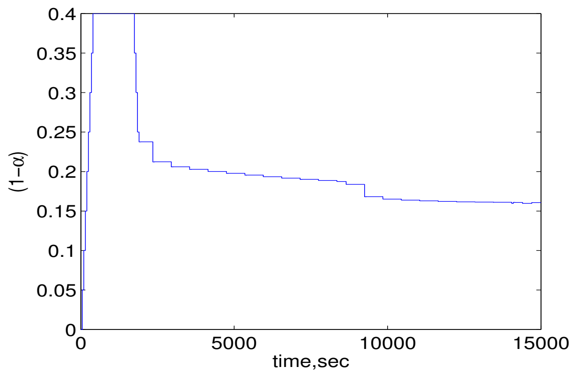


Fig. 6. trajectory of the manipulated variable: fraction of total mass flow of hot gas that is extracted

state where the minimum temperature at the at the inlet of the catalytic sections is above the threshold value. Figure 7(c) shows the optimal fraction of total mass flow of hot gas that is extracted to achieve the desired control performance. The optimal value is now higher than the value obtained in Figure 6 and this is expected since the plant includes the effect of the external heat transfer resistant that is given by the insulation. By simulations (not shown) we observed that the oscillations in the adjustments of the manipulated variable can be decreased by increasing the number of discrete points in the controller ($m$). However, a finer discretization comes at a higher computational load.

## 4. CONCLUSION

In this paper we presented the formulation of a controller to a distributed parameter flow system with periodic oscillation of the flow direction. The controller uses the Model Predictive Control concept and is based on the Model Predictive control

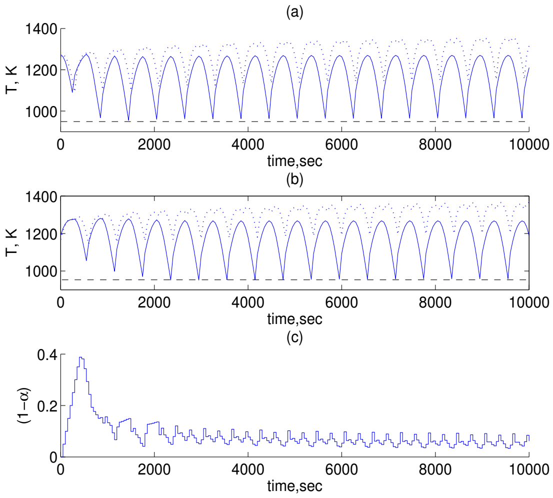


Fig. 7. (a) Temperature at point $C_1$ (see Figure 2) with control (solid line) and without control (dotted line). (b) Temperature at point $C_2$ (see Figure 2) with control (solid line) and without control (dotted line). The dashed line indicates the temperature lower bound.(c) Trajectory of the manipulated variable: fraction of total mass flow of hot gas that is extracted

scheme for convection-dominated distributed parameter systems proposed by Shang *et al.* (2004). We applied the control scheme to a CFRR unit for the combustion of methane to maximize the amount of energy that can be extracted from the reactor without extinguishing the reaction.

Simulations are used to show the ability of the controller to find the optimal extraction of hot gas extraction while keeping the minimum temperature at the inlet of the active catalyst sections above a minimum threshold value that guarantee stable operation (no deactivation of catalyst sections).

## NOMENCLATURE

$v_s$ superficial velocity $(m/s)$
$\alpha$ fraction of total inlet mass flow in the reactor (-)
$k_m$ mass transfer coefficient $(m/s)$
$a_v$ surface area per unit volume $(m^2/m^3)$
$h$ heat transfer coefficient
$\rho$ density $(kg/m^3)$
$Cp$ heat capacity $(J/kg \cdot K)$
$k_r$ first-order rate constant $(s^{-1})$
$\eta$ effectiveness factor
$\Delta H$ enthalpy of reaction of methane $(J/mol)$
$H_P$ prediction horizon
$H_C$ control horizon
$T_{sampling}$ sampling time
$m$ number of discrete points in the controller

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