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OPTIMIZING ADAPTIVE CALORIMETRIC MODEL PREDICTIVE CONTROL OF A BENCHMARK SEMI-BATCH REACTION PROCESS

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Abstract: Application of optimization based techniques in control and operational optimization schemes of semi-batch batch reaction processes allow the rigorous inclusion of economic as well as safety aspects. For a restricted class of reaction processes, the on-line optimization problem can be reduced to optimization on a short prediction horizon requiring only crude process models. This paper extends an earlier approach of Helbig *et al.* (1998) of simultaneous temperature control and feed rate optimization in the framework of model predictive control (MPC). Based on simple calorimetric process models, the given MPC formulation is readily applicable in typical industrial multi-product/multi-purpose plants. The major capability of driving the process along constraints is illustrated in a simulation study of an isothermal semi-batch reaction process with a single reaction.

Keywords: Dynamic Optimization, Model Predictive Control, Batch Reactor, Safety

1. INTRODUCTION

Batch and semi-batch reaction processes are of high importance in the manufacturing of fine chemicals, pharmaceuticals, specialties, polymers and other high value products. Industrial batch production ranges from flexible multi-product plants for small-volume products up to large dedicated-equipment plants for certain polymers. Being intrinsically dynamic, batch reaction processes offer a wide application area for dynamic optimization techniques (Bonvin *et al.*, 2001).

However, the number of industrial applications of rigorous model based optimization in batch reactor control and operation is still very limited. The typical requirement to provide a process model capable of predicting process dynamics over the entire batch is a major reason for this observation. Especially in multi-product/multi-purpose plants the derivation of detailed physico-chemical reaction models for each of the products can not be afforded. Furthermore, only simple measurements like temperatures and pressures rather than component concentrations are available on-line, defining a typical industrial "minimal process knowledge situation".

Within this work, an on-line optimization scheme specifically tailored to this situation is presented, which treats simultaneous temperature control and on-line feed rate optimization for semi-batch single reaction processes in the framework of Model Predictive Control (MPC).

2. PRINCIPLE OF OPTIMIZING MPC SCHEME

The basic principle of calorimetric MPC schemes for the optimization of semi-batch reaction processes is to use available degrees of freedom on the process (i.e. the feed rate) in order to reduce the batch time while simultaneously solving a classical temperature control problem. For a restricted class of reactions this approach leads to optimal operation of batch processes without the necessity

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to accurately predict process behavior to the end of the batch. The underlying transformation of an endpoint-optimization problem ("minimize batch time") into a local optimization problem naturally transforms the optimization task into a problem, interpreted by Helbig *et al.* (2000) as a specific form of so called direct optimization schemes for operational optimization of general transient processes.

The transformation of global into local optimization problems is obviously not possible in all cases. Specifically, the transformation of batch endpoint constraints into local MPC constraints is generally infeasible. An industrial relevant process class, however, exists, for which the overall transformation is straightforward. This class comprises isothermal semi-batch reaction processes with single reactions and without endpoint constraints. The task is to drive this single reaction to a certain degree of reactant conversions which defines the end of the batch.

As already shown in a case study of a two-phase polymerization reactor (Helbig *et al.*, 1998), simple process models based on the principles of reaction calorimetry (Schuler and Schmidt, 1992) are sufficient in order to solve the problem. Calorimetric state estimation techniques can be applied in order to permanently adapt crude models to match current process dynamics and thus allowing at least short horizon predictions, even in cases of large structural and parametric uncertainties.

Design of an optimizing MPC scheme consists of three crucial elements: First, an appropriate *cost function* has to be chosen which drives the process along different active constraints. For the above type of reaction process, this can be achieved by extending the classical MPC controller objective function for temperature control with an additional term maximizing the feed rate. Second, a suitable calorimetric *estimator* has to be derived in order to infer unknown inputs, parameters and states from available measurements. Input estimation in (linear) energy balances is the preferred structure, leading to equations like

$$\ldots \frac{\mathrm{d}T}{\mathrm{d}t} = Q_R + \ldots \ , \tag{1}$$

in which the unknown input Q_R may be estimated on the basis of simple trend models:

$$\frac{\mathrm{d}Q_R}{\mathrm{d}t} = 0 \ . \tag{2}$$

Finally, *prediction models* for the estimated variables (e.g. Q_R) have to be formulated. The application of the simple estimation model may be restricted by controllability issues in cases where the estimated variable represents important process variables depending on the manipulated variables. Therefore a specific *prediction model differing from the estimation model* is often inevitable.

The example below contains several types of trend models and uncertainty predictions for an application case, in which the prediction model covers both reaction and cooling system dynamics.

3. BENCHMARK SEMI-BATCH REACTION PROCESS

The benchmark control and optimization problem described in the sequel has been derived at Bayer AG, Leverkusen. For secrecy reasons no real product, plant, and production data may be revealed. Therefore, an "anonymous" semi-batch reaction process model is presented which contains control relevant aspects of a number of existing production processes using a similar type of equipment. Major characteristics are the inclusion of a cooling system model and a safety related path constraint into the optimization problem. Figure 1 shows a schematic of the reactor with the main instrumentation. A full model description of the benchmark process along with detailed information about the expected uncertainties and ranges for parameter variations is given elsewhere (Cruse *et al.*, 2001).

3.1 *Process description*

The benchmark process describes a simple reaction system $A + B \rightarrow C + D$ where A and B are the reactants, C is the desired product and D is a by-product. The exothermic liquid-phase reaction is carried out within a solvent S and requires a catalytic component *cat*. The reactor is initially filled with a fixed amount of A, S, and *cat* at ambient temperature and pressure. After the initial reactor content has been heated to the required reaction temperature, feeding of a B-S mixture starts and the reaction phase begins. For this control study, the end of the batch is defined by a specified conversion of B.

The reactor is coupled to a jacket in which a fixed amount of cooling medium is recirculated. Temperature control of the reactor content can be achieved by manipulating the temperature of the recirculating medium. For this purpose, either hot or cold medium may be inserted into the loop through equal percentage control valves. A similar amount to that inserted is automatically withdrawn from the recycle loop.

An additional safety scenario is included, which covers a cooling system breakdown by constraining the maximum temperature reached by an adiabatic conversion of the reactor content (Helbig *et al.*, 1998).

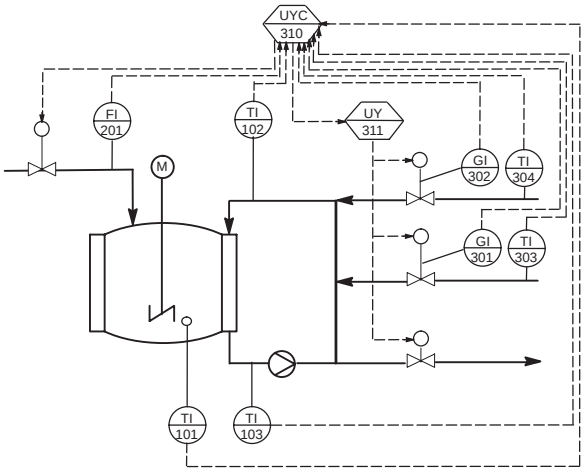

Fig. 1. Reactor schematic.

3.2 *Control and optimization task*

In this benchmark problem three operational phases can be distinguished: (1) the heating phase, (2) the reactant feeding phase, and (3) a final reaction phase lasting until the conversion is reached. Phases (2) and (3) together are referred to as reaction phase. The reactor is initially filled with $8100\,kg$ of component A, $19700\,kg$ solvent and $35\,kg$ catalyst. Temperatures at the beginning of phase (1) are assumed to be ambient temperature, i.e 25^0C for the reactor temperature T_R, the jacket inlet temperature $T_{J,i}$, and the jacket outlet temperature $T_{J,o}$.

The control and optimization system utilizes the split range variable C_{con} and the feed rate $\dot{M}_f$ as manipulated variables. The first task is to heat the initial reactor content from ambient temperature to the required reaction temperature of 70 ^{0}C and to tightly keep temperature at this value during the subsequent reaction phase. Feeding may only start after the reaction temperature has been reached. A total amount of 5000 kg has to be fed during the reaction phase. At the beginning of the reactant feeding phase the feed rate is constrained by a linear increase of the feed rate starting from 100 kg/h to 1000 kg/h within half an hour. The batch ends when B has been converted up to a remaining amount of 50 kg.

A suitable feeding strategy has to be determined which allows tight temperature control during the reaction and which keeps the adiabatic end temperature T_{ad}^{max} below 85 ^{0}C (path constraint). The optimization task is to minimize the duration of the reaction phase.

3.3 *Nominal optimal solution*

Figure 2 shows results obtained from dynamic optimization of the full model using the software package DYNOPT (1999), jointly developed by Lehrstuhl für Prozesstechnik and Bayer AG.

In order to illustrate how changes of the operational region of a manipulated variable can influence the sequence of active constraints and thus the structure of the solution, two cases with different upper limits of the allowable feed rate have been treated. In Case I, only 1000 kg/h are allowed. As can be seen from the left part of Figure 2, the capacity of the cooling system is not limiting the duration of the reaction phase in this case. The active constraint during reaction switches from feed rate to adiabatic maximum temperature. In Case II, the maximum feed rate is 2000 kg/h. This changes the solution structure, since the lower cooling constraint becomes active shortly after the beginning of the feeding phase. In case II the optimal feed rate is no longer determined by its constraints as proposed by Bonvin *et al.*, (2001). This problem often arises in multi-product/multi-purpose plants due to limitations in the utility systems even if the structure of the reaction system does not change and no conflicting influences of the feed on the reaction system is present. Therefore, from our perspective on-line optimization is the method of choice in most industrial applications.

3.4 *Benchmark problem*

An on-line control system has to be designed for cases I and II which is capable of

- quickly heating up the reactor content without temperature overshoot,
- keeping temperature deviations from set-point smaller than 1 ^{0}C during reaction, and
- minimizing reaction time by adding the feed as quickly as possible, obeying the constraints on manipulated variables and T_{ad}^{max}.

The controller may use the following on-line measurements only: Reactor temperature T_R (T101), jacket inlet temperature $T_{J,i}$ (T102), jacket outlet temperature $T_{J,o}$ (T103), temperatures of cold (T304) and hot (T303) medium, current valve positions (G302) and (G301), and the current feed rate (F201).

With respect to the available process knowledge, three different *scenarios* should be treated. First, a nominal predictive controller should be designed which may exploit the full model (1). Second, robustness tests should be carried out introducing both model plant mismatch and measurement errors (2). Finally, a controller should be designed assuming reaction kinetics to be unknown. The latter scenario defines a typical "minimum knowledge" situation (3).

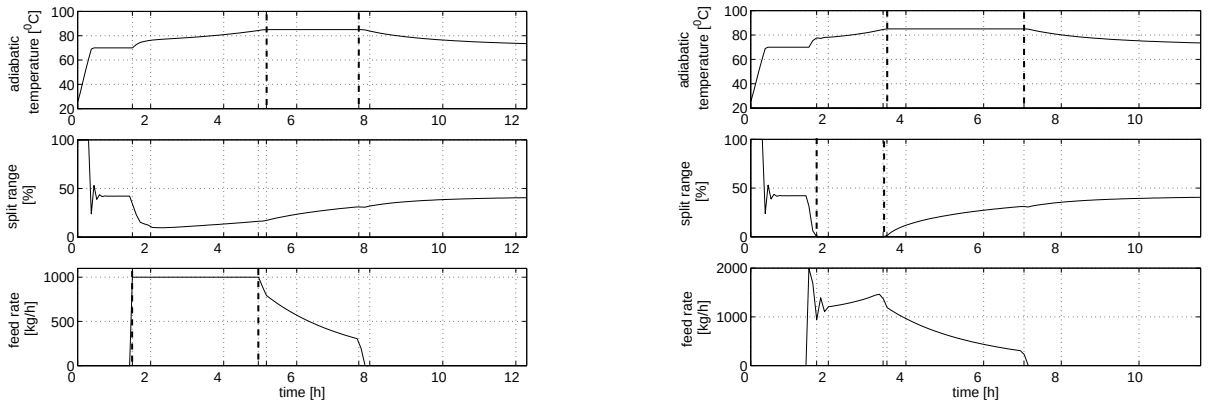

Fig. 2. Nominal optimal solution: Manipulated variables and T_{ad}^{max}. Left: Case I, Right: Case II.

4. MPC SIMULATION STUDY

In the sequel, design of an optimizing calorimetric predictive controller coupled to an Extended Kalman Filter (EKF) is discussed. The design is intended to solve the nominal benchmark problem as well as scenarios with varying degrees of process knowledge. The study solely focuses on the reaction phase, since a temperature setpoint trajectory is utilized for the initial heating phase.

4.1 *EKF model*

Calorimetric state estimation and prediction model update is based on the following model applied in an Extended Kalman Filter (EKF) with bounded outputs according to Vallière and Bonvin, (1989):

Mass and component balances:

$$\frac{\mathrm{d}M_R}{\mathrm{d}t} = \dot{M}_f\,, \tag{3}$$

$$\frac{\mathrm{d}M_A}{\mathrm{d}t} = \frac{\dot{Q}_R}{\Delta H_R} MW_A \cdot 3.6\,, \tag{4}$$

$$\frac{\mathrm{d}M_B}{\mathrm{d}t} = w_{B,f}\dot{M}_f + \frac{\dot{Q}_R}{\Delta H_R} MW_B \cdot 3.6\,. \tag{5}$$

Energy balance for the reactor content:

$$M_R c_{p,R} \frac{\mathrm{d}T_R}{\mathrm{d}t} = \Big([\dot{Q}_R + (\alpha_0 + \Delta\alpha)\, M_R/M_{R,0} \\ (0.5\,(T_{J,o} + T_{J,i}) - T_R)] \cdot 3600 \\ + \dot{M}_f c_{p,f}\,(T_f - T_R) \Big)\,. \tag{6}$$

Energy balance of jacket content:

$$\frac{\mathrm{d}T_{J,o}}{\mathrm{d}t} = \frac{1}{(M_J c_{p,c})} \Big(\dot{M}_c c_{p,c}\,(T_{J,i} - T_{J,o}) \\ - (\alpha_0 + \Delta\alpha)\, M_R/M_{R,0} \\ (0.5\,(T_{J,i} + T_{J,o}) - T_R) \cdot 3600)) \,. \tag{7}$$

Energy balance for the cooling/heating utility:

$$\frac{\mathrm{d}T_{J,i}}{\mathrm{d}t} = \Big(\Delta\dot{Q}_C \cdot 3600 + \dot{M}_c c_{p,c}\,(T_{J,o} - T_{J,i}) \\ + \dot{Q}_{S,cold} \Big[1 + VT_{cold} \\ \left(\frac{K_{V0}^{cold}}{K_{VS}^{cold}} \exp\left(\log\left(\frac{K_{VS}^{cold}}{K_{V0}^{cold}} \right) C_{cold} \right) \right)^2 - 1 \Big]^{0.5} \\ (c_{p,cold} T_{cold} - c_{p,c} T_{J,o}) \\ + \dot{Q}_{S,hot} \Big[1 + VT_{hot} \\ \left(\frac{K_{V0}^{hot}}{K_{VS}^{hot}} \exp\left(\log\left(\frac{K_{VS}^{hot}}{K_{V0}^{hot}} \right) C_{hot} \right) \right)^2 - 1 \Big]^{0.5} \\ (c_{p,hot} T_{hot} - c_{p,c} T_{J,o}) \Big) / (M_M c_{p,c})\,. \tag{8}$$

Split range for the valve positioning:

$$C_{cold} = \begin{cases} 100 - 2C_{con}\,, & \text{if } C_{con} < 50 \\ 0\,, & \text{if } C_{con} \geq 50 \end{cases} \tag{9}$$

$$C_{hot} = \begin{cases} 2\,(C_{con} - 50)\,, & \text{if } C_{con} > 50 \\ 0\,, & \text{if } C_{con} \leq 50 \end{cases}\,. \tag{10}$$

Trend models for error terms:

$$\frac{\mathrm{d}\Delta\alpha}{\mathrm{d}t} = 0\,, \tag{11}$$

$$\frac{\mathrm{d}\Delta\dot{Q}_C}{\mathrm{d}t} = 0\,, \tag{12}$$

$$\frac{\mathrm{d}\dot{Q}_R}{\mathrm{d}t} = 0\,. \tag{13}$$

The uncertainties in the jacket heat transfer are handled by estimating a drifting parameter $\Delta\alpha$. This corresponds to the assumption that the coefficient for the initially filled reactor is known rather well. The complex terms in Eqn. (8) arise due to the consideration of the valve behavior described by equal percentage valves. Uncertainties in these valve flows lead to a non-zero error term $\Delta\dot{Q}_C$, which is assumed to be constant over the prediction horizon (Eqn. 12).

4.2 *MPC model*

The optimization task is to minimize the duration of the reaction phase which is equal to the minimization of the reactant feeding phase. The following type of cost function may be applied:

$$\Phi = \alpha_1 \sum_{i=1}^{N} (T_{R_i} - T_{R_i}^{set})^2 + \alpha_2 \sum_{i=1}^{N} (C_{con_i} - C_{con_{i-1}})^2 + \alpha_3 \sum_{i=1}^{N} (\dot{M}_{f_i} - \dot{M}_{f_{i-1}})^2 - f_J \,. \quad (14)$$

It comprises four terms representing the temperature control task, penalties on controller moves, and a free customizable fourth term. In this application the feed rate depending fourth term is evaluated continuously $f_J = -\alpha_4 \int_t^{t+t_h} \dot{M}_f dt$. Here $t_h = N \cdot \Delta t$ is the prediction horizon with Δt being the sampling interval used for control and N the number of prediction steps.

In the most streamlined version, the prediction model for the MPC comprises all model equations of the EKF model. If, however, the estimated variable represents an important process variable with high dependency on the manipulated variables (i.e. the heat of reaction), a specific prediction model structure $\dot{Q}_R = f_Q(p_Q, ...)$ may be proposed for prediction. The initial value of the prediction should match the current estimate, which can be achieved by updating some parameter p_Q or assuming a constant error term over time.

In cases with only parametric uncertainties in the kinetic model (benchmark scenario 2), the trend model structure is used with the algebraic reaction kinetic model given by

$$f_Q = -V_R * \Delta H_R K_{R,0} \exp\left(\frac{-EA_R}{R_{gas}\,(T_R + 273.15)}\right) \left(\frac{M_{cat} \cdot 1000}{MW_{cat} V_R}\right) \left(\frac{M_A \cdot 1000}{MW_A V_R}\right) \left(\frac{M_B \cdot 1000}{MW_B V_R}\right) \frac{1}{60} \,,$$

with the volume of the reactor content

$$V_R = \frac{M_R}{\rho_R} \,. \quad (15)$$

In this approach, the full kinetic model structure is used in order to predict the future values of the heat of reactions, starting from the current EKF estimate.

For scenario 3, a different approach has to be chosen. Since the reaction is isothermal, the major prediction aspect with respect to the heat of reaction covers the dependency on the feed component B. Assuming the reaction to be locally first order with respect to B, the following alternative (algebraic) trend model can be formulated:

$$\dot{Q}_R = k_Q \cdot M_B \;\; \text{with} \;\; k_Q = \dot{Q}_{R_{EKF}} / M_B \,. \quad (16)$$

In this case, prediction of $\dot{Q}_R$ starts at the current EKF estimate, too.

In order to handle the safety constraint the MPC model also contains an equation to predict the adiabatic maximum temperature T_{ad}^{max}, which is constrained over the reaction phase.

Numerical calculations have been carried out applying the recently completed on-line version of the DYNOPT package. Within DYNOPT-online, f_J can be freely customized and may be extended e.g. by soft constraints on certain variables.

4.3 *Simulation results*

For all simulation studies a sampling interval Δt of 2 minutes and a prediction horizon of 24 minutes ($N = 12$) has been chosen. The weighting factors α_2 and α_3, penalizing control moves, have been set to zero. For the heating phase, a smooth setpoint temperature trajectory from 25 ^{o}C to 70 ^{o}C has been applied such that the required reaction temperature is reached after 1.5 h. At that point, the reaction phase starts.

The results of a robustness test of the MPC are depicted in Figures 3, where a 10 % error in the reaction kinetic parameters has been introduced. Results are comparable to those in the nominal case. Similar results can be obtained if reaction kinetics are assumed to be unknown and Eqn. (16) is applied for prediction.

In any case, the quality of the calorimetric estimation is crucial for the obtainable control results. Since errors in the heat of reaction are integrated in the mass balances, prediction of T_{ad}^{max} is also subject to unavoidable integral errors (see Figure 4). As the constraint on T_{ad}^{max} is active for a long time, feed optimization results will suffer significantly from erroneous predictions of this interfered process variable.

5. CONCLUSIONS

It has been shown that the proposed optimizing adaptive calorimetric MPC scheme is capable of solving the combined temperature control and feed rate optimization problem of the benchmark semi-batch reaction process. The same solution structure with respect to active constraints as compared to the nominal optimal solution has been derived by the proposed model predictive

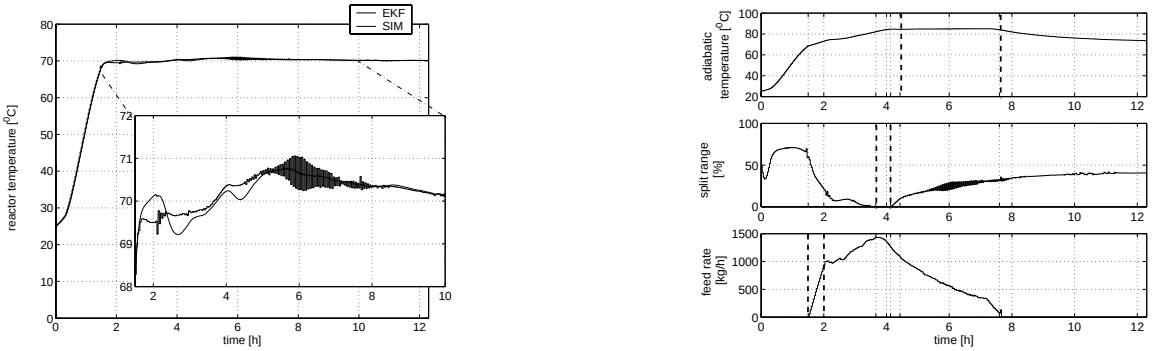

Fig. 3. MPC with model plant mismatch, Case II. Left: reactor temperature, right: Feed rate, cooling capacity, and T_{ad}^{max}

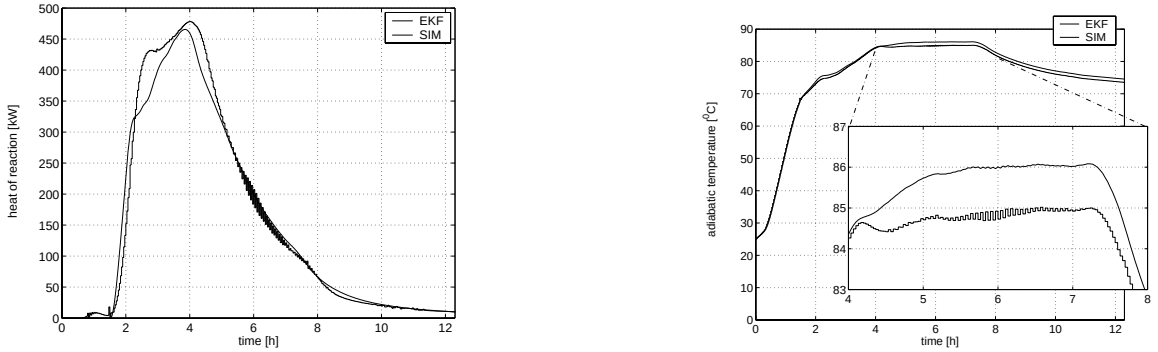

Fig. 4. Estimation and prediction error in MPC with model plant mismatch, Case II. Left: heat of reaction, right: T_{ad}^{max}.

controller. The switching structure of active constraints as a reaction to variations of the allowed operational range of the manipulated variables can easily be handled by the on-line optimizing model predictive controller, which is of particular interest in multi-purpose/multi-product plants.

The given controller formulation also covers the solution for scenarios 2 and 3 of the benchmark problem with increasing model uncertainties. Due to lack a of space, results with respect to these scenarios have been restricted to a robustness test with parametric errors in the kinetic model. This case has been selected since it matches with an application case of the proposed MPC scheme at Bayer AG, Leverkusen. The calorimetric MPC for a realistic industrial reactor has been implemented and tested in simulation and at the real plant. Results from field tests and details of a flexible implementation concept will be the subject of a forthcoming communication.

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