Prediction of the ledge thickness inside a high-temperature metallurgical reactor using a virtual sensor

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Abstract. A non-intrusive inverse heat transfer procedure for predicting the time-varying thickness of the phase-change ledge on the inner surface of the walls of a high-temperature metallurgical reactor is presented. An extended Kalman filter with augmented state is coupled with a nonlinear state-space model of the reactor in order to estimate on-line the position of the phase front. The data are collected by a heat flux sensor located inside or outside of the reactor wall. This non-intrusive method can be seen as a virtual sensor which is defined as the combination of an estimation algorithm with measurements for the estimation of ‘hard to measure’ on-line process variables. The inverse prediction of the ledge thickness with the virtual sensor is thoroughly tested for typical operating conditions that prevail inside an industrial facility. Due to the fact that the melting/solidification process inside the reactor is highly nonlinear, results show that the accuracy of the state-space identification and the virtual sensor estimation is far superior when a nonlinear state-space model and the extended Kalman filter are employed, as opposed to a linear state-space model and the classic Kalman filter. In the former, it is shown that the discrepancy between the exact and the estimated ledge thickness remains smaller than 10% at all times.

1. Introduction
An interesting melting/solidification phenomenon that arises in high-temperature metallurgical reactors such as electric arc furnaces, blast furnaces and aluminium electrolysis cells is the formation of solid layers, sometimes called ledges or banks, on the inner surface of the reactor walls (Fig. 1). This ledge is formed as the molten material comes into contact with the cooled surface of the wall and solidifies. The presence of the ledge is highly desirable. It serves as a protective barrier against the corrosive molten material, thereby maintaining the integrity of the cell and prolonging its active life. On the other hand, too thick a ledge is detrimental to the reactor as the active cell volume is reduced. Moreover, in electrolysis cells, horizontal currents may be generated thereby disturbing the magneto-hydrodynamics stability of the cell and, as a result, decreasing the current efficiency [1]. Maintaining a ledge of optimal size at all times is therefore crucial for the safe and profitable operation of the metallurgical reactor.
Unfortunately, due to the hostile conditions that prevail inside the reactor, probing the time-varying thickness and shape of the ledge with sensors submerged into the molten material is a very difficult task, not to say impractical. The standard method for measuring the thickness of the ledge is to probe it manually [2]. This method is time consuming and requires qualified personnel to perform the task. Also, the measurements are usually taken days apart and they require the opening of the reactor which results in significant heat losses to the surroundings and the release of undesirable chemicals into the atmosphere.

The alternative is to attempt to predict the ledge profile with inverse heat transfer methods that rely on thermal measurements taken from sensors located in the reactor walls. This non-intrusive method can be seen as a virtual sensor, or soft sensor, defined as the combination of an estimation algorithm with measurements that allows the estimation of ‘hard to measure’ on-line process variables.

The present article is organized as follows. First, a finite-difference model (FDM) is developed for predicting the nonlinear melting/solidification process inside the reactor (detailed model). Second, a nonlinear state-space model (NSSM) of the reactor, more computationally efficient than the FDM, is presented (reduced model). Third, the inverse method (the virtual sensor), combining an extended Kalman filter and the NSSM is shown. The virtual sensor enables to estimate the ledge thickness from heat flux measurements taken inside or outside of the reactor walls. Finally, the inverse prediction of the ledge thickness with the virtual sensor is thoroughly tested for typical operating conditions that prevail inside an industrial facility.

2. Finite-difference model of the metallurgical reactor (detailed model)

The one-dimensional phase change problem under investigation is depicted in Fig. 2. A time-varying ledge of thickness $s(t)$, which corresponds to the solidification front location, is built against the inner surface of a brick wall of thickness $L$. The outer surface of the brick wall, i.e. the left boundary condition, is cooled by forced convection heat transfer with an impinging air jet where the air temperature $T_\infty$ and the heat transfer coefficient $h$ are perfectly known and remain constant. A time-varying heat flux $q''_w(t)$, which represents the heat load supplied to the reactor, is imposed on the right boundary condition at $x=L+D$. 

Based on the assumptions reported in Ref. [3], the governing heat diffusion equation for the wall and the PCM may be stated as:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \delta H \frac{\partial F}{\partial t}$$

(1)

The boundary conditions are:

$$k \frac{\partial T}{\partial x} \bigg|_{x=0} = h(T(0,t) - T_w)$$

(2)

$$k \frac{\partial T}{\partial x} \bigg|_{x=L+D} = q_m(t)$$

(3)

and the initial condition is

$$T(x,0) = T_0(x)$$

(4)

The second term on the right-hand side of Eq. (1) accounts for the solid/liquid phase change. Of course, this term vanishes inside the brick wall. The liquid fraction $F$ varies linearly between the solidus temperature $T_{sol}$ and the liquidus temperature $T_{liq}$ in the following manner:

$$F = F(T) = \begin{cases} 0 & T \leq T_{sol} \\ \frac{T - T_{sol}}{T_{liq} - T_{sol}} & T_{sol} < T < T_{liq} \\ 1 & T \geq T_{liq} \end{cases}$$

(5)

Eqs. (1-5) were discretized using second-order finite differences in space, and first-order differences in time with an implicit scheme. The resulting set of algebraic equations is then solved using a tri-
diagonal matrix algorithm (TDMA). For each time step, the liquid fraction $F$ in Eq. (1) is determined iteratively according to the enthalpy method proposed by Voller and Swaminathan [4]. Thus, with the known conditions (Eqs. 2-5), the FDM provides the evolution of the temperature field $T(x,t)$, the heat flux distribution $q''(x,t)$, and the ledge thickness $s(t)$. The above FDM was thoroughly tested and validated using analytical solutions and results available in the open literature. Further details concerning the validation of the numerical model are reported in Ref. [3].

3. Nonlinear state-space model of the metallurgical reactor (reduced model)

In the last decades, the popularity of model reduction techniques have increased significantly in various fields such as heat transfer, fluid mechanics, solid mechanics, and process control. The main objective of these methods is to extract, from knowledge of the physical process (simulations or experimental data), a low-dimensional system (reduced model) that has nearly the same response characteristics as the process under study. The idea behind model reduction is the need, in many instances, for a simplified model that captures the main features of the original complex model. The simplified model, much more computationally efficient, may then be used in place of the original complex model, either for simulations or for control applications [5].

Since the inverse method used in the current work is composed of an extended Kalman filter, state-space models were a more convenient choice for building the reduced model. The nonlinear state-space identification thus consists in casting the predictions of the FDM, considered here as the exact values, into the following nonlinear discrete state-space form:

\[
x[k + 1] = f(x[k], u[k]) + w[k]
\]

\[
y[k] = g(x[k]) + v[k]
\]

$y = [ q''_{\text{met}} \ s ]^T$ is the measurement vector. It contains the information extracted from the FDM, that is the heat flux measurement $q''_{\text{met}}$ and the ledge thickness $s$. $x=[x_1 \ x_2]^T$ is the state vector, with no physical meaning. $u$ is the input vector which is equivalent to the input heat flux $q''_u$ (Eq. 3). $v$ is the sensor noise which is considered as a zero mean Gaussian white noise with covariance $R$ defined as the covariance matrix of the measurement noise, $w$ is the process noise which accounts for the disturbances to the metallurgical reactor dynamics. It is assumed once again to be a zero mean Gaussian white noise with covariance $Q$ defined as the covariance matrix of the process noise. Finally, $k$ corresponds to the sampling instant.

Given the input vector $u$ and the corresponding measurement vector $y$, the objective of the state-space identification is to compute the nonlinear functions $f$ and $g$ that minimize the cost function $V_N$ defined as:

\[
V_N = \sum_{k=1}^{N} \epsilon^2[k] = \sum_{k=1}^{N} (y[k] - \hat{y}[k])^2
\]

where $\epsilon$ is the difference between the measurement vector $y$ (extracted from the FDM) and the predicted output of the state-space model $\hat{y}$, and $N$ is the total number of sampling instants. In order
to compute the nonlinear functions $f$ and $g$, the state-space identification algorithm relies on the iterative prediction-error minimization method (PEM) reported in reference [6].

The usefulness of the present state-space identification procedure is exemplified in the following case. The heat flux measurement $q''_{mes}$ is taken at the brick/ledge interface ($x=L$) while the input vector $u$ corresponds to typical values for the heat load inside high-temperature reactors. The corresponding predictions of the nonlinear state-space model (NSSM) are compared in Fig. 3. For comparison, a linear state-space model (LSSM) is also shown in this figure. It is seen that the agreement between the predictions of the NSSM and those of the FDM is excellent, i.e. the relative root-mean-square error (RRMSE) values remain lower than 3% for the heat flux and ledge thickness predictions.

![Figure 3: Predictions of the FDM versus that of the linear (LSSM) and nonlinear (NSSM) state-space models.](image)

4. Inverse method for estimating the ledge thickness (virtual sensor)

In the inverse problem, the heat flux $q''_{in}(t)$ on the right boundary is unknown (Fig. 4). It may be estimated however with an inverse method which employs a heat flux sensor embedded into the brick wall or placed on its outside surface. Once the heat flux $q''_{in}(t)$ has been estimated based on these measurements $q''_{mes}(t)$, the solidification front location, or ledge thickness, $s(t)$ is determined from the nonlinear state-space model (NSSM) of section 3. A schematic of the overall inverse methodology based on the extended Kalman filter and the NSSM is provided in Fig. 5.

![Figure 4: Schematic of a 1-D inverse phase change problem inside a metallurgical reactor.](image)
Figure 5: The inverse method: an extended Kalman filter coupled with a nonlinear state-space model. It acts as a virtual sensor for estimating the ledge thickness.

The first part of the virtual sensor is composed of the extended Kalman filter (EKF), one of the most popular nonlinear versions of the well-known linear Kalman filter. The EKF is a set of mathematical equations that provide an efficient recursive mean to estimate the nonlinear state of a process (the phase change process). In the current work, the EKF uses an augmented state that corresponds to the unknown input signal \( q'' \) in. Eqs. 6-7 are then modified using this new state vector defined as \( X = [x_1, x_2, q'' \text{ in}]^T \).

\[
X[k + 1] = f(X[k]) + w[k] \tag{9}
\]
\[
y[k] = g(X[k]) + v[k] \tag{10}
\]

In order to estimate correctly the process states, the EKF proceeds through two steps: 1) the time update step (prediction) followed by 2) the measurement update step (correction). The time update equations project the current state estimate \( \hat{X}[k|k] \) and the error covariance matrix estimate \( P[k|k] \) forward in time in order to obtain the a priori estimate for the next time step, i.e. \( \hat{X}[k + 1|k] \) and \( P[k + 1|k] \) (Eqs. 11-12).

\[
\hat{X}[k + 1|k] = A[k|k] \hat{X}[k|k] \tag{11}
\]
\[
P[k + 1|k] = A[k|k] P[k|k] A[k|k]^T + Q \tag{12}
\]

The covariance matrices \( P[k|k] \) and \( P[k + 1|k] \) characterize the accuracy of the computed state estimate \( \hat{X}[k|k] \) and \( \hat{X}[k + 1|k] \) respectively, and the matrix \( A[k|k] \) corresponds to the jacobian of the nonlinear function \( f \) (Eq. 9). The feedback is then performed by the measurement update equations that incorporate a new measurement \( \tilde{q}' \) mes into the a priori estimates \( \hat{X}[k + 1|k] \) and \( P[k + 1|k] \) in order to obtain an improved a posteriori estimate \( \hat{X}[k + 1|k + 1] \) and \( P[k + 1|k + 1] \) (Eqs. 13-14).
\[
\dot{X}[k+1|k+1] = \dot{X}[k+1|k] + K[k]Q_{\text{meas}}[k] - C[k+1|k]X[k+1|k] \\
P[k+1|k+1] = (I - K[k]C[k+1|k])P[k+1|k]
\]

(13)

(14)

where \( I \) is the identity matrix, \( K \) is the Kalman gain (Eq. 15) that minimizes the a posteriori error covariance \( P[k+1|k+1] \), and the matrix \( C[k+1|k] \) is the jacobian of the nonlinear function \( g \) (Eq.10)

\[
K[k] = P[k+1|k]C[k+1|k]^T\left(C[k+1|k]P[k+1|k]C[k+1|k]^T + R\right)^{-1}
\]

(15)

From the unknown input heat flux \( \hat{q}_m^- \) given by the extended Kalman filter, i.e. \( \hat{q}_m^- = \hat{X}[0 \ 0 \ 1] \), the ledge thickness can be calculated with the nonlinear state-space model of section 3 (Eqs. 6-7)

\[
x[k+1] = f(x[k], \hat{u}[k])
\]

(16)

\[
\hat{s}[k] = g(x[k])[0 \ 1]
\]

(17)

where \( \hat{u} = \hat{q}_m^- \) is a new input vector, and \( \hat{s} \) is the estimated ledge thickness. The above inverse heat transfer procedure was thoroughly tested for estimating the time-varying input heat flux \( q''_m(t) \) on the right boundary and therefore for predicting the time-varying thickness of the ledge inside a reactor. The corresponding time-varying exact (FDM) and predicted (inverse method) ledge thicknesses are compared in Fig. 6. Once again, the prediction of the inverse method using a linear Kalman filter (KF) is added for comparison.

Figure 6: Exact (FDM) and predicted (inverse method) ledge thicknesses using the linear Kalman filter (KF) and the nonlinear extended Kalman filter (EKF).
Fig. 6 shows that the discrepancy between the exact and the estimated ledge thickness remains smaller than 10% and gives a maximum error of $2.5 \times 10^{-3}$ m, which is smaller than the uncertainty associated with the manual probing method [3]. Finally, Fig. 6 shows that the linear inverse method using the Kalman filter cannot achieve the same performance level than its nonlinear counterpart due to the fact that it cannot take in account the nonlinear behavior of the melting/solidification process inside the reactor.

5. Concluding remarks

A non-intrusive inverse heat transfer procedure for predicting the time-varying thickness of the phase-change ledge on the inner surface of the walls of a high-temperature metallurgical reactor was presented. An extended Kalman filter with augmented state was coupled with a nonlinear state-space model of the reactor in order to estimate on-line the position of the phase front. The data were collected by a heat flux sensor located inside or outside of the reactor wall. This non-intrusive method can be seen as a virtual sensor defined as the combination of an estimation algorithm with measurements that allows to estimate ‘hard to measure’ on-line process variables. The inverse prediction of the ledge thickness with the virtual sensor was thoroughly tested for typical operating conditions that prevail inside an industrial facility. Due to the fact that the melting/solidification process inside the reactor is highly nonlinear, results showed that the accuracy of the state-space identification and the virtual sensor estimation is far superior when a nonlinear state-space model and the extended Kalman filter were employed, as opposed to a linear state-space model and the classic Kalman filter. In the former, it was shown that the discrepancy between the exact and the estimated ledge thickness remained smaller than 10% at all times.

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