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Bang-bang control and singular arcs in reservoir flooding

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Abstract

Over the past few years, dynamic optimization of reservoir flooding using optimal control theory has received significant attention. Various studies have shown that dynamic (time-varying) injection and production settings can yield a higher Net Present Value (NPV) than conventional reactive settings. In these studies, the optimization procedure itself is always gradient-based, where the gradients are obtained with an adjoint formulation. However, the shape of the optimal injection and production settings is generally not known beforehand. The main contribution of this paper is to investigate why and under what conditions reservoir flooding problems can be expected to have bang-bang (on–off) optimal solutions. A major practical advantage of bang-bang controls is that they can be implemented with simple on–off valves. Furthermore, there are sufficient optimality conditions that are tailor-made for bang-bang solutions, meaning we can actually check whether a solution is locally optimal or not. These results are illustrated by a water flooding example of a 3-dimensional reservoir in a fluvial depositional environment, modeled with 18.553 grid blocks. The valve settings of 8 injection and 4 production wells are optimized over the life of the reservoir, with the objective to maximize NPV. It turns out that optimal settings are sometimes bang-bang, and sometimes bang-bang in combination with so-called singular arcs. For the latter situations, however, bang-bang solutions are found that are only slightly suboptimal.

Keywords: Optimal control; Bang-bang control; Singular arcs; Reservoir flooding

1. Introduction

1.1. Reservoir flooding as optimal control problem

A whole variety of reservoir flooding problems can be formulated as optimal control problems, where the goal is to find a control u over a time interval $[0, T]$ that maximizes a certain performance measure $J(u)$. What distinguishes an optimal control problem from a static optimization problem is that u drives a dynamical system, often described by differential equations together with an initial condition, whose subsequent state trajectory determines $J(u)$.

In reservoir flooding, the controls are often combinations of injection rates, production rates, bottom-hole pressures, concentrations and/or valve-settings, while the performance measure is often Net Present Value (NPV). The dynamical system is of course a reservoir.

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Over the past few years, dynamic optimization of reservoir flooding using optimal control theory has received significant attention. Various studies have shown that dynamic (time-varying) injection and production settings can yield a higher NPV than conventional reactive settings. However, there are two reasons why finding optimal solutions to reservoir flooding problems is particularly challenging.

1. A reservoir model has nonlinear dynamics, and it is therefore not possible to find an analytical solution.
2. A reservoir model is often extremely large-scale, and it therefore takes a long time to evaluate $J(u)$. For example, there can be more than 10^6 states whose trajectories require several hours to compute.

For large-scale nonlinear optimal control problems, the most common approach to finding optimal solutions is to parameterize the control and, starting from an initial parameter guess, iteratively improve upon it until the first order necessary conditions for a local optimum are satisfied — Athans (1966), Stengel (1986). Virtually all the studies on dynamic optimization of reservoir flooding in the literature are based on such an iterative scheme.

1.2. Literature review

Asheim (1987, 1988) consider optimizing individual injection and production rates in water flooding. Ramirez and Fathi (1984), Fathi and Ramirez (1984, 1986, 1987) consider optimizing injection concentrations in chemical flooding. Mehos and Ramirez (1989) consider optimizing the production bottom-hole pressure and the injection rates of water and CO_2 in CO_2 flooding. Liu et al. (1993) consider optimizing the rate and steam quality of an injector and the bottom-hole pressure of a producer in steam flooding.

Even though the particular applications in these studies vary, they have much in common. The goal is always to maximize NPV, while the gradients of NPV with respect to the controls are computed using an adjoint model.[1] Furthermore, the shapes of the optimal solutions turn out to be smooth (*i.e.* gradually varying; continuously differentiable), but it is not clear why.

Sudaryanto and Yortsos (2000, 2001) consider maximizing water breakthrough time in water flooding by optimizing two injection rates. However, in contrast to the previously mentioned literature, they state that the optimal solution is a bang-bang control — meaning that over the entire time interval, each component of u takes on either its minimum or maximum value. Consequently, they disregard the possibility of smooth optimal solutions and only consider bang-bang controls, parameterized in terms of switching times (times at which a component of the control switches from one extreme value to the other).

In light of this work, the subsequent studies Brouwer (2004) and Brouwer and Jansen (2004), which consider optimizing individual rates and valve settings in water flooding, are particularly interesting. They find that the optimal rates are smooth, but that the optimal valve settings are sometimes bang-bang — even though they do not parameterize the control in terms of switching times. No explanation is given as to the discriminating factor.

1.3. Main contribution and outline of paper

The main contribution of this paper is to investigate why and under what conditions reservoir flooding problems can be expected to have bang-bang optimal solutions.

A major practical advantage of bang-bang controls is that they can be implemented with simple on–off valves. Furthermore, there exist sufficient optimality conditions that are tailor-made for bang-bang solutions. We can therefore guarantee whether a solution is locally optimal or not, which is not possible with necessary conditions only.

As a prerequisite for later sections, Section 2 shows that many reservoir flooding problems are in fact linear in the control (but nonlinear in the state), meaning that both the differential equations governing the dynamics of the reservoir model and the to-be-optimized performance measure depend linearly on the control. Then, why and under what conditions such problems sometimes have bang-bang optimal solutions is clarified in Section 3, where second order sufficient optimality conditions are also summarized. Several techniques to exploit this knowledge in an optimization procedure are given in Section 4. Finally, in Section 5, these results are illustrated by a water flooding example of a three dimensional oil–water reservoir containing 12 wells, modelled with 18.553 grid blocks. This work is a further extension of the preliminary results in Zandvliet et al. (2006), and forms part of a larger research project to enable closed-loop model-based reservoir management through combining model-based optimization with frequent model updating — Brouwer et al. (2004), Jansen et al. (2005). Here we only consider optimization without changing the model parameters over time.

[1] Adjoint models are discussed in Section 3.

2. Reservoir flooding problems linear in the control

2.1. Reservoir models linear in the control

The common method for numerical modelling of fluid flow through porous media is combining a mass balance equation with Darcy's Law, which states that flow is proportional to a pressure gradient — Peaceman (1977), Aziz and Settari (1979). Almost all reservoir simulators are based on this paradigm. This section shows that the resulting differential equations governing fluid flow in a reservoir are linear in the control.

To be specific, we will consider the flow of oil and water through a slab of porous media and ignore several important modelling aspects — such as the presence of a gas phase, gravity effects, aquifers, and rock compressibility. It will be shown, however, that the resulting differential equations are still linear in the control if these aspects are included — only the derivation is lengthier.

The mass balances for oil (o) and water (w) are[2]

$$\frac{\partial}{\partial t}(\phi\rho_i S_i) = -\nabla\cdot(\rho_i \bar{u}_i) - q_i, \quad i \in \{\mathrm{o},\mathrm{w}\} \tag{1}$$

where t is time, $\nabla\cdot$ the divergence operator, ϕ the porosity, ρ_i the density of the phase i, $\bar{u}_i$ the superficial velocity, and S_i the saturation. Finally, q_i is a source/sink term which will be discussed later.

Conservation of momentum is governed by the Navier–Stokes equations, but is normally simplified for low velocity flow through porous media to be described by the semi-empirical Darcy's equation — Hubbert (1956):

$$\bar{u}_i = -k\frac{k_{\mathrm{r}i}}{\mu_i}\nabla p_i, \quad i \in \{\mathrm{o},\mathrm{w}\} \tag{2}$$

where p_i is the pressure of phase i, ∇ the gradient operator, k the absolute permeability, $k_{\mathrm{r}i}$ the relative permeability, and μ_i the viscosity of phase i. Note that k_{rw} and k_{ro} are highly dependent on the water saturation S_{w} (they can generally vary between 0 and 1) and thus form a major source of nonlinearity.

Substituting Eq. (2) into Eq. (1) leads to two flow equations with four unknowns: p_{o}, p_{w}, S_{o} and S_{w}. Two additional equations are required to complete the system description. The first is the closure equation requiring that the sum of the phase saturations equals one:

$$S_{\mathrm{o}} + S_{\mathrm{w}} = 1. \tag{3}$$

[2] To be precise we would have to include spatial coordinates, such as Cartesian ones (**x**, **y**, **z**). For notational convenience, however, all of the dependent arguments are omitted, *i.e.* we write $\bar{u}_i$ instead if $\bar{u}_i(t, \mathbf{x}, \mathbf{y}, \mathbf{z})$ and ϕ instead if $\phi(\mathbf{x}, \mathbf{y}, \mathbf{z})$.

Second, the relation between the individual phase pressures is given by the capillary pressure p_{cow}, which is assumed to be a function of water saturation. We can therefore write

$$p_{\mathrm{w}} = p_{\mathrm{o}} - p_{\mathrm{cow}}. \tag{4}$$

Common practice in reservoir simulation is to substitute Eqs. (3) and (4) into the flow equations by taking the oil pressure p_{o} and water saturation S_{w} as state variables, leading to

$$\frac{\partial}{\partial t}(\phi\rho_{\mathrm{o}}[1-S_{\mathrm{w}}]) = \nabla\cdot(\tilde{\lambda}_{\mathrm{o}}\rho_{\mathrm{o}}\nabla p_{\mathrm{o}}) - q_{\mathrm{o}} \tag{5}$$

$$\frac{\partial}{\partial t}(\phi\rho_{\mathrm{w}}S_{\mathrm{w}}) = \nabla\cdot\left(\tilde{\lambda}_{\mathrm{w}}\rho_{\mathrm{w}}\nabla p_{\mathrm{o}} - \tilde{\lambda}_{\mathrm{w}}\rho_{\mathrm{w}}\frac{dp_{\mathrm{cow}}}{dS_{\mathrm{w}}}\nabla S_{\mathrm{w}}\right) - q_{\mathrm{w}} \tag{6}$$

where $\tilde{\lambda}_{\mathrm{o}} = k\frac{k_{\mathrm{ro}}}{\mu_{\mathrm{o}}}$ and $\tilde{\lambda}_{\mathrm{w}} = k\frac{k_{\mathrm{rw}}}{\mu_{\mathrm{w}}}$ are the fluid mobilities. It is assumed that there is no flow across the boundaries of the reservoir geometry over which Eqs. (5) and (6) are defined, other than through the source/sink terms q_{o} and q_{w} (Neumann boundary conditions).

Because oil and gas reservoirs are generally heterogenous (their geological properties vary significantly over space), Eqs. (5) and (6) cannot be solved analytically, but must be evaluated numerically. The first step in this numerical evaluation is spatial discretization, where the reservoir is divided into a finite number of "grid blocks", whose geological properties are assumed to be homogenous.

Recall that each grid block relates to two states: oil pressure and water saturation. Let us stack all of these states into a vector x and all of the source terms into a vector q

$$x = \left[p_{\mathrm{o}}^1 \ldots p_{\mathrm{o}}^N \; S_{\mathrm{w}}^1 \ldots S_{\mathrm{w}}^N\right]^T, \tag{7}$$

$$q = \left[q_{\mathrm{o}}^1 \; q_{\mathrm{w}}^1 \ldots q_{\mathrm{o}}^N \; q_{\mathrm{w}}^N\right]^T. \tag{8}$$

The Eqs. (5) and (6) for each of the N grid blocks are, after some manipulation, replaced by a single equation of the form

$$\frac{d}{dt}V(x) = \tilde{T}(x) - q, \quad x(0) = x_0, \tag{9}$$

where x_0 is the initial condition — see Aziz and Settari (1979) for more details. Because a reservoir has evolved over millions of years, it is initially in equilibrium. In other words, the fluids in a reservoir only start to flow once wells are drilled.

If an injector well is perforated in grid block j, then we can directly control the source terms q_o^j and q_w^j. Usually, only water (and not oil) is injected to keep the pressure in the reservoir above a certain level, and we can write

$$q_w^j = \frac{\rho_w}{\mathbf{v}^j} q^j, \tag{10}$$

$$q_o^j = 0, \quad j \in \mathcal{N}_{\text{inj}} \tag{11}$$

where $\mathbf{v}^j$ is the volume of grid block j, q^j is the rate of injected fluid, and $\mathcal{N}_{\text{inj}}$ the set of indices in which there is an injector location.

On the other hand, if a producer well is perforated in grid block j, then we can only indirectly control the source terms q_o^j and q_w^j, since the produced liquid is a combination of oil and water:

$$q_w^j = \frac{\rho_w}{\mathbf{v}^j} f_w^j q^j, \tag{12}$$

$$q_o^j = \frac{\rho_o}{\mathbf{v}^j}(1 - f_w^j) q^j, \quad j \in \mathcal{N}_{\text{prod}} \tag{13}$$

where q^j is the rate of produced fluid, $f_w^j = \frac{\tilde{\lambda}_w^j}{\tilde{\lambda}_w^j + \tilde{\lambda}_o^j}$ is the fractional flow rate of water, and $\mathcal{N}_{\text{prod}}$ is the set of indices in which there is a producer location.

The q^j terms are related to the pressure in the well by a so-called well model

$$q^j = \alpha^j w^j (p_o^j - p_{\text{bh}}^j), \quad j \in \{\mathcal{N}_{\text{inj}}, \mathcal{N}_{\text{prod}}\} \tag{14}$$

where p_{bh}^j is the well's bottom-hole pressure, and α^j a control valve setting (simply a multiplication factor ranging from 0 to 1). The well index w^j contains the well's geometric flow factors and rock and fluid properties of the reservoir directly around the well.

The $\frac{d}{dt}V(x)$ term in Eq. (11) can be expanded as $\tilde{V}(x)\dot{x}$, with $\tilde{V}(x)$ invertible as long as the fluids are compressible — see the Appendix. Substituting Eqs. (10)–(14) into Eq. (9) and pre-multiplication by $\tilde{V}^{-1}(x)$ then leads to a model of the form

$$\dot{x}(t) = f_1(x(t), t) + f_2(x(t), t)u(t), \quad x(0) = x_0. \tag{15}$$

Here, we assume that the control u represents one of the following: q^j, α^j or p_{bh}^j. The situation that we can control both α^j and p_{bh}^j individually does not fit into the form Eq. (15), since this would involve the product of two controls. The additional time arguments in f_1 and f_2 can be used to represent time-varying properties, such as skin factor.

We stress that it is not necessary to actually perform this transformation when implementing Eqs. (9)–(14) in a reservoir simulator; our only is goal is to show that it could be done. Furthermore, it could also be done when considering:

— the presence of a gas (g) phase, since q_i still enters Eq. (1) linearly for $i \in \{\text{o, w, g}\}$,
— gravity effects, since this only requires an additional term in the right-hand side of Eq. (2),
— aquifers, since they can be viewed as source terms q_w in Eq. (1) over which we have no control,
— rock compressibility, since this only complicates the expansion of $\frac{d}{dt}V(x)$ into $\tilde{V}(x)\dot{x}$ as shown in the Appendix.
— multi-phase flow in wells using lift tables, where the tubing head pressure is the control.

2.2. Performance measures linear in the control

As mentioned earlier, a common economical performance measure is simple Net Present Value, defined as the total oil revenues minus the total injection and production costs over a time interval [0, T], in combination with a discount factor d. Letting r_{oil} denote oil revenue per unit volume, r_{inj} the injection cost per unit volume, and r_{prod} the water production cost per unit volume, we can write

$$J_{\text{npv}}(u) = \int_0^T \Bigg[\underbrace{\sum_{j \in \mathcal{N}_{\text{prod}}} r_{\text{oil}}(t)[1 - f_w^j(t)]q^j(t)}_{\text{oil revenue}} - \underbrace{\sum_{j \in \mathcal{N}_{\text{prod}}} r_{\text{prod}}(t) f_w^j(t) q^j(t)}_{\text{production cost}} + \underbrace{\sum_{j \in \mathcal{N}_{\text{inj}}} r_{\text{inj}}(t) q^j(t)}_{\text{injection cost}} \Bigg] \times \underbrace{\frac{1}{(1 + d(t))^t}}_{\text{discount factor}} (dt). \tag{16}$$

Another commonly used performance measure is the sweep efficiency $J_{\text{se}}(u)$, which is the total amount of oil "swept" away by fluid injection. This can naturally be expressed in terms of the water saturations at the terminal time T. Letting $\mathcal{N}_{\text{tot}}$ denote the set of all grid blocks in our model, we can write

$$J_{\text{se}}(u) = \sum_{j \in \mathcal{N}_{\text{tot}}} S_w^j(T). \tag{17}$$

Both Eqs. (16) and (17) are performance measures of the form

$$J(u) = \psi(x(T),T) + \int_0^T \{l_1(x(t),t) + l_2(x(t),t)u(t)\}dt \tag{18}$$

where $u(t)$ enters the integrand of Eq. (18) linearly. The additional time arguments in l_1 and l_2 can be used to represent time-varying properties, such as volatile oil prices and interest rates.

2.3. Constraints

In most applications there will be constraints on both the states and controls. For the moment, however, we only consider upper and lower bounds on the individual components of the control. In other words, for a control with m components we require that $u(t)$ be in the following set

$$\mathcal{U} := \{z \in \mathbb{R}^m : u_{\min} \le z \le u_{\max}\} \tag{19}$$

for given $u_{\min}$ and $u_{\max} \in \mathbb{R}^m$ for all $t \in [0, T]$.

Furthermore, the terminal time T in Eq. (18) is considered to be fixed. Of course in practice T is an important decision variable and, in contrast to u, it need not be constrained. In Section 3 we will show how to deal with such free terminal time problems.

To summarize:

The considered class of reservoir flooding problems are in fact optimal control problems of the following form.

Problem 1:

$$\begin{aligned} &\text{maximize } \psi(x(T),T) + \textstyle\int_0^T \{l_1(x(t),t) + l_2(x(t),t)u(t)\}dt \\ &\text{subject to } \dot{x}(t) = f_1(x(t),t) + f_2(x(t),t)u(t) \\ &\qquad x(0) = x_0 \\ &\qquad u(t) \in \mathcal{U}\ \forall\ t \in [0,T] \\ &\qquad \mathcal{U} = \{z \in \mathbb{R}^m : u_{\min} \le z \le u_{\max}\}. \end{aligned}$$

3. Theory of bang-bang control

3.1. Necessary conditions for optimality

In this section we show that the optimal solution to Problem 1 can be expected to be a bang-bang control by first considering a more general problem, namely

Problem 2:

$$\begin{aligned} &\text{maximize } \psi(x(T),T) + \textstyle\int_0^T l(x(t),u(t),t)dt \\ &\text{subject to } \dot{x}(t) = f(x(t),u(t),t) \\ &\qquad x(0) = x_0 \\ &\qquad u(t) \in \mathcal{U}\ \forall\ t \in [0,T] \\ &\qquad \mathcal{U} = \{z \in \mathbb{R}^m : u_{\min} \le z \le u_{\max}\} \end{aligned}$$

and deriving first order necessary condition for optimality.

The basic reasoning behind deriving these conditions is that, given a candidate optimal control u, the first order variation of the performance measure should be non-positive for "small" variations of u. These derivations are given in virtually all textbooks on optimal control. See for example Athans and Falb (1966), Bryson and Ho (1975), Luenberger (1981) and Stengel (1986).

A common approach is to define an auxiliary function, the so-called Hamiltonian, as follows

$$\begin{aligned} H(x(t),u(t),\lambda(t),t) := {} & l(x(t),u(t),t) \\ & + \lambda^T(t) f(x(t),u(t),t). \end{aligned} \tag{20}$$

The vector $\lambda(t) \in \mathbb{R}^{2N}$ is often referred to as the adjoint, co-state, Lagrange multiplier or tangent vector.

We define a new function v which is allowable (meaning $v(t) \in \mathcal{U}\ \forall\ t \in [0, T]$) and close to u, in the sense that

$$\sum_{i=1}^{m} \int_{t=0}^{T} |u_i(t) - v_i(t)| dt < \varepsilon \tag{21}$$

for some small $\varepsilon > 0$. It can be shown that if λ satisfies the adjoint system equation

$$\dot{\lambda}(t) = -\frac{\partial H^T}{\partial x}(x(t),u(t),\lambda(t),t) \tag{22}$$

with terminal time condition

$$\lambda(T) = \frac{\partial \psi^T}{\partial x}(x(T),T) \tag{23}$$

the effect on the performance measure is

$$\begin{aligned} J(v) - J(u) &= \int_{t=0}^{T} \{H(x(t),v(t),\lambda(t),t) - H(x(t),u(t),\lambda(t),t)\}dt \\ &\quad + o(\varepsilon) \end{aligned} \tag{24}$$

in which $o(\varepsilon)$ denotes terms of smaller order than ε.

A first order necessary condition for $J(v)-J(u)$ to be nonpositive is that

$$H(x(t),\bar{v},\lambda(t),t) \leq H(x(t),u(t),\lambda(t),t),\ \forall\ \bar{v}\in\mathcal{U},\forall\ t\in[0,T]. \tag{25}$$

This result is referred to as Pontryagin's Maximum Principle and it is one of the most important results in optimal control theory — see Pontryagin et al. (1962).

An important observation is that, for Problem 1, these necessary conditions have a particular structure. Let us define

$$\beta(t) := l_2(x(t),t) + \lambda^T(t)f_2(x(t),t). \tag{26}$$

The necessary condition (25) then becomes

$$\beta(t)\bar{v} \leq \beta(t)u(t)\ \forall\ \bar{v}\in\mathcal{U},\forall\ t\in[0,T]. \tag{27}$$

Note that f_1 and l_1 do not enter Eq. (27). This necessarily leads to the following form of the components of u

$$u_i(t) = \begin{cases} u_{\min,i}, \text{if } \beta_i(t)<0 \\ u_{\max,i}, \text{if } \beta_i(t)>0 \end{cases} \tag{28}$$

for $i=1,\ldots,m$. $\beta\in\mathbb{R}^{1\times m}$ is often understandably referred to as the switching function and its zeros the switching times. Note that $\frac{\partial H}{\partial u}=\beta$ and that $\frac{\partial^k H}{\partial u^k}=0$ for $k\geq 2$. Loosely speaking, the component β_i at time t can therefore be viewed as the first order variation of J due to a small change in the component u_i at time t.

For clarity, we emphasize that the control u determines the state x through Eq. (15), that the pair (x, u) determines the adjoint through Eqs. (22) and (23), and that the pair (x, λ) determines the switching function β through Eq. (26). The control satisfies the first order necessary optimality conditions (25) if the zeros of the components of β coincide with the times that the components of u are discontinuous — as illustrated in Fig. 1. How to actually compute such a control u is discussed in Section 4.

If the switching function contains only isolated zeros as in Fig. 1, the problem is said to be regular. On the other hand, if any component of β is zero along an open time interval, the problem is said to be singular, and such an interval is called a singular arc. The difficulty lies in the fact that, along the singular arc, Eq. (25) no longer provides information since the first order variation of J is then insensitive to variations in u.

In short, any locally optimal solution to a reservoir flooding problem that can be written as Problem 1 is necessarily a bang-bang control, possibly in combination with singular arcs.

This is not surprising, as it is in line with the intuitive notion that in a locally optimal solution of a static optimization problem, either the derivative vanishes or the to-be-optimized parameters are on the boundary of the feasible set. However, the following is surprising.

Pure bang-bang controls (ones without singular arcs) are widely encountered as optimal strategy for optimal control problems that can be written as Problem 1.

Some examples from other application fields where pure bang-bang controls are shown to be optimal include:

- minimum-time problems for linear systems — Bellman (1956),
- minimum-time problems for bilinear systems — Mohler (1973),
- optimal control of batch reactors — Blakemore and Aris (1962),
- optimal thermal control — Belghith et al. (1986),
- optimal drug administration in cancer chemotherapy — Ledzewicz and Schattler (2002).

According to the previously mentioned studies by Sudaryanto and Yortsos, Brouwer and Jansen, and the example treated in Section 5, it now seems that pure bang-bang controls are also sometimes (but not always) encountered as optimal strategy for reservoir flooding problems that can be written as Problem 1.

3.2. Remarks

3.2.1. State constraints

It is now clear why we only consider upper and lower bounds on the individual components of the control u: the step from Eqs. (27) to (28) in the derivation of bang-bang optimal control does not apply to problems involving more general (in)equality constraints on the control.

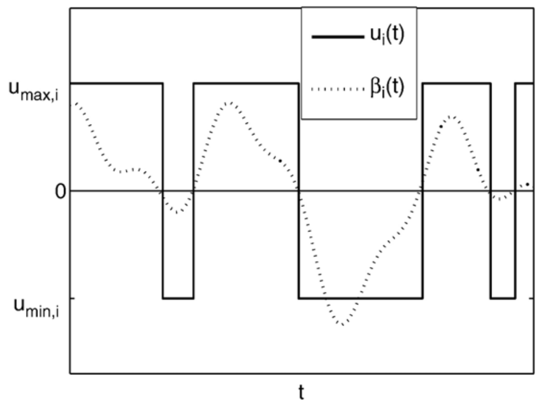

Fig. 1. The ith component of the scaled switching function β_i and the corresponding bang-bang control u_i.

In fact, this is precisely the reason why the optimal rates in Brouwer (2004) and Brouwer and Jansen (2004) are smooth, while the optimal valve settings are sometimes bang-bang: there are additional equality constraints on the rates in order to balance total injection with total production, but not on the valve settings.

In practice, more general (in)equality constraints on the control can be relevant (for example balancing the total injection and production rates), as can state constraints (for example keeping the pressure in the reservoir below a fracturing threshold, and above the bubble-point pressure). Unfortunately, optimal control problems with state constraints are, in general, difficult to solve. Some progress in handling state constraints in reservoir flooding problems has recently been achieved by Sarma et al. (2005, 2006), and Kraaijevanger et al. (2007).

3.2.2. Free terminal time problems

If the terminal time T is free, the so-called transversality condition

$$\frac{\partial \psi}{\partial T}(x(T),T)+H(x(T),u(T),\lambda(T),T)=0 \tag{29}$$

must be added to the set of necessary conditions for optimality — see Stengel (1986).

3.2.3. Locally optimal vs. globally optimal solutions

Since Problem 1 is a nonlinear (or more importantly: nonconvex) optimization problem due the nonlinear dynamics of Eq. (15), we cannot guarantee that a locally optimal solution is also a globally optimal solution. If an optimization scheme converges to the same solution for different initial conditions, we might have more confidence that that particular solution is indeed globally optimal — but we generally cannot prove it.

3.2.4. Smoothness

Throughout this paper, we assume that f_1, f_2, l_1, l_2 and ψ are continuously differentiable with respect to x and t — see for example Eq. (22). In general, this is a reasonable assumption in reservoir flooding problems. For example, f_1 and f_2 are continuously differentiable as long as (k_{rw}, k_{ro}) depend smoothly on S, and (μ_{rw}, μ_{ro}, ρ_{w}, ρ_{o}) depend smoothly on p. For nonsmooth problems, the reader is referred to Clarke (1983). It also is worthwhile to point out that the $\frac{\partial f}{\partial x}$ term in Eq. (22) is almost always available in a fully-implicit reservoir simulator — Sarma et al. (2005).

3.2.5. Continuous vs. discrete-time problems

The trajectory x can generally not be solved analytically for given u and x_0, and the same applies to λ. Consequently, Eqs. (15) and (22) are discretized in time and u is often taken to be piece-wise constant (*i.e.* step-like). Although there is also a discrete-time version of Pontryagin's Maximum Principle, a similar treatment would require too much space. We therefore only remark that the conditions are largely similar to the continuous-time case. See Bryson and Ho (1975) for more details.

3.2.6. Well configuration

We only consider reservoir flooding problems with a fixed configuration of wells. In practice, however, the number and location of wells are important decision variables. Furthermore, it is also possible to drill new wells during the life of a reservoir. Taking any of these possibilities into consideration greatly complicates matters, since this leads to so-called mixed integer problems which are generally much more difficult than the problems considered in this paper. See Bangerth et al. (2006) for an overview and Yeten et al. (2003) and Aitokhuehi et al. (2004) for some recent progress in this direction.

3.3. Sufficient conditions for optimality

To ensure that a control u satisfying the first order necessary conditions given in the previous subsection is indeed a locally optimal solution to Problem 1, second order sufficient conditions must be verified. Many authors have been involved with deriving higher-order conditions, both necessary and sufficient, for optimality — see for example Krener (1973), Bressan (1985) and Kawski (2003). Recently, however, second order sufficient conditions specifically for pure bang-bang solutions have been derived in Agrachev et al. (2002), and their efficient numerical implementation discussed in Maurer et al. (2005). The reader is referred to these two works (and the references therein) for proofs, as we will only state the main results.

In order to use the sufficient optimality conditions in Agrachev et al. (2002), we must make four assumptions:

(a) the terminal time T is fixed,
(b) the bang-bang control u satisfies the necessary optimality conditions and is regular (has no singular arcs), and
(c) only one component of u switches at any particular time.

Given n distinct switching times $t_k \in [0,T]$ with $t_1 < \ldots < t_n$, let us define the bang-bang vector τ as

$$\tau = [t_1 \ldots t_n]^T. \tag{30}$$

Furthermore, let τ determine a bang-bang control u. Due to assumptions (b) and (c), the components of τ coincide with the zeros of the components of the switching function. That is, for each $k=1,\ldots, n$ there is a unique index $i(k)$ such that only the component $u_{i(k)}$ is discontinuous at t_k, and only the component $\beta_{i(k)}$ is zero at t_k.

Our fourth and final assumption is that(d) the strict bang-bang property holds

$$\frac{d}{dt}\beta_{i(k)}(t_k)(u^{k+1}_{i(k)}-u^{k}_{i(k)})>0, k=1,\ldots,n \tag{31}$$

where $u^k_{i(k)}$ denotes the value of $u_{i(k)}(t)$ for $t_{k-1}<t<t_k$.

With this notation, $\left(u^{k+1}_{i(k)}-u^{k}_{i(k)}\right)$ represents the "jump" of $u_{i(k)}(t)$ at the switching time t_k. Loosely speaking, Eq. (31) therefore requires that $u_{i(k)}(t)$ actually switches from one value to another at $t=t_k$. Note that since u satisfies Pontryagin's Maximum Principle Eq. (27), the left hand side of Eq. (31) is always larger than or equal to zero — we simply require it to be strictly larger than zero.

The performance measure J is now a function of τ. Surprisingly, the only condition that we now need to verify is whether the Hessian $\frac{\partial^2 J}{\partial \tau^2}(\tau)\in\mathbb{R}^{n\times n}$ is negative definite

$$\frac{\partial^2 J}{\partial \tau^2}(\tau)<0. \tag{32}$$

If we have found a τ such that u satisfies the first order necessary conditions for optimality, we can only conclude that u might be a locally optimal solution to Problem 1. However, if τ also satisfies Eq. (32), we can make the much stronger statement that u is a locally optimal solution. We stress that "optimal" here refers to variations of u satisfying Eq. (21) (*i.e.* optimal with respect to the so-called $\mathcal{L}_1$-norm).

If $\frac{\partial^2 J}{\partial \tau^2}(\tau)$ is negative semi-definite, u again might be a locally optimal solution, whereas if it is indefinite it certainly is not. Whatever the situation, Eq. (32) is clearly a simple condition to check. This is illustrated in the example of Section 5.

4. Exploiting the bang-bang property

4.1. Steepest descent method

As mentioned earlier, the Eqs. (15) and (22) are always discretized in time, and u is often taken to be piece-wise constant (*i.e.* step-like). Let u be divided into K equal intervals over $[0, T]$, let $\mathbf{u}^k_j\in\mathbb{R}^m$ denote the value of $u(t)$ over the j-th interval in the k-th iteration, and let

$$\mathbf{u}^k=[\mathbf{u}^k_1\ldots\mathbf{u}^k_K]^T. \tag{33}$$

An optimal solution to Problem 1 is then usually found by iteratively improving upon an initial choice of $\mathbf{u}^k$ in a steepest descent[3] method

$$\tilde{\mathbf{u}}^{k+1}=\mathbf{u}^k+s^k\frac{dJ^T}{d\mathbf{u}^k}(\mathbf{u}^k), \tag{34}$$

$$\mathbf{u}^{k+1}=\max(u_{\min},\min(u_{\max},\tilde{\mathbf{u}}^{k+1})) \tag{35}$$

where Eq. (35) is to make sure that $\mathbf{u}^{k+1}$ leads to an allowable control (*i.e.* one that satisfies Eq. (19)). Here, s_k is the step size and $\frac{dJ}{d\mathbf{u}^k}$ the (total) derivative of J, whose components are given by

$$\frac{\partial J}{\partial \mathbf{u}^k_{j,i}}(\mathbf{u}^k)=\int_{t=(j-1)T/K}^{jT/K}\frac{\partial H^T}{\partial u_i}(x(t),u(t),\lambda(t),t)dt. \tag{36}$$

for $j=1,\ldots, K$ and $j=1\ldots,m$. Although it has the obvious advantage of being easy to implement, the steepest descent method is known for its slow convergence near an optimal solution. There are other methods that have better convergence properties, but they are not considered here.

4.2. Switching time methods

If we assume that the optimal solution to Problem 1 is a bang-bang control, we can in principle very efficiently parameterize the control in terms of switching times. An optimal solution can then be found by iteratively improving upon an initial choice of the switching times, for example again using a steepest descent method. There are several methods to compute optimal bang-bang controls which focus on finding the optimal number and value of switching times, such as

- the Switching–Time–Variation Method (STVM) of Mohler (1973),
- the method of Glashoff and Sachs (1977),
- the Switching Time Optimization (STO) of Meier and Bryson (1990),
- the Switching Time Computation of Lucas and Kaya (2001).

A major challenge, however, is that the optimal number of switching times is not known beforehand. For regular optimal control problems involving linear nth-order systems, it has been proven that the optimal

[3] This is a slight abuse of terminology since, strictly speaking, it is only a "steepest" descent method if there are no active constraints on $\mathbf{u}^k$.

solution has at most n switching times — see Bellman (1956) and Athans and Falb (1966). In Sussmann (1979), these results have been extended to problems involving nonlinear systems. Unfortunately, they are not of much practical use, since in our intended application n is in the order of 10^4–10^6.

In all of the previously mentioned methods, the initial number of switching times is therefore guessed. In light of this drawback we propose the following alternative descent method, which is a slight alteration of Eqs. (34) and (35).

4.3. Alternative descent method

Choose an initial bang-bang control $\mathbf{u}^k$, and iteratively improve upon it in the following descent method

$$\mathbf{u}_{j,i}^{k+1} = \mathbf{u}_{j,i}^{k} + h_{j,i}^{k}\mathrm{sign}\left(\frac{\partial J}{\partial \mathbf{u}_{j,i}^{k}}(\mathbf{u}^k)\right),$$

$$h_{j,i}^{k} = \begin{cases} u_{\max,i}-u_{\min,i} & \text{if } j,i \text{ is in } \Omega_1^k \\ 0 & \text{if } j,i \text{ is not } in\ \Omega_1^k \end{cases}$$

$$\Omega_1^k = \text{set of indices of } \tilde{s}^k \text{ largest components of } \Omega_2$$

$$\Omega_2^k = \text{set of } \left|\frac{\partial J}{\partial \mathbf{u}_{j,i}^{k}}(\mathbf{u}^k)\right| \text{ for which } \mathbf{u}_{j,i}^{k} \text{ is not aligned with } \frac{\partial J}{\partial \mathbf{u}_{j,i}^{k}}(\mathbf{u}^k). \tag{37}$$

Roughly speaking, this amounts to abruptly switching the $\tilde{s}^k$ most important components of $\mathbf{u}^k$ that are not yet aligned as in Fig. 1 from one lower/upper bound to the other, until either the set Ω_2^k is empty (and the solution satisfies the necessary optimality conditions) or there is no more improvement (and the solution is suboptimal). $\tilde{s}^k$ can be viewed as the step size. The advantage of this method is that it does not work with switching times, while $\mathbf{u}^k$ (and thereby u) is still a bang-bang control at each iteration and can therefore be implemented with simple on–off valves.

5. Example

5.1. Description of reservoir flooding problem

We consider a water flooding example of a 3-dimensional oil–water reservoir in a fluvial depositional environment. It is modeled with 18.553 grid blocks of dimension 20 m×20 m×20 m, and there are 7 vertical layers. Fig. 2 depicts the absolute permeability field, together with the location of 12 vertical wells. The modeling is as in Section 2, but with gravity effects. Geological and fluid properties are given in Table 1 — the reservoir geometry and values for the absolute permeability field can be obtained by contacting the corresponding author. The relative permeability curves are depicted in Fig. 3.

The well specifications are as follows:

- Each well is available as of time $t=0$.
- Each well is vertical, and is perforated in all 7 layers of the reservoir.
- Each well operates at constant bottom-hole pressure. For the 8 injectors, the bottom-hole pressure is set to 415 bar at the lowest perforation. For the 4 producers, the bottom-hole pressure is set to 390 bar at the highest perforation. The pressures in the other perforations are computed assuming hydrostatic equilibrium in the wellbore.
- Each well is equipped with a single valve, whose setting can vary between 10^{-6} (a lower bound of 0 leads to numerical problems) and 1. In other words,

$$\mathcal{U} := \{z\in\mathbb{R}^{12} : 10^{-6} \le z_k \le 1, k = 1, \ldots, 12\}.$$

- The valve setting of a well applies to all 7 perforations.
- The well indices w^j are computed using a Peaceman model with a wellbore radius of 0.1m and zero skin factor.

The initial pressure in the reservoir is computed assuming hydrostatic equilibrium, with the top of the reservoir at a depth of 4000 m and at a pressure of 400 bar.

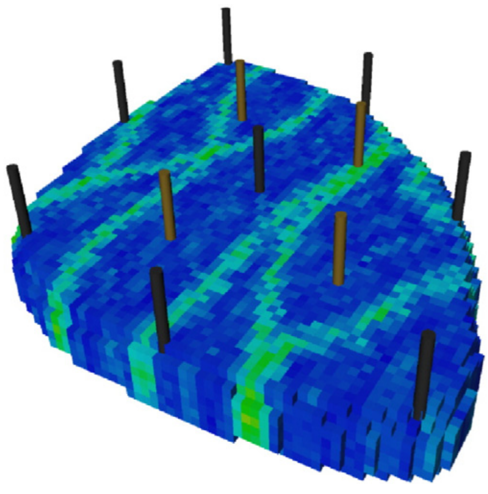

Fig. 2. Absolute permeability field, with 8 injectors (dark) and 4 producers (light).

Table 1
Values of geological and fluid properties

Symbol	Value	Unit
ϕ	0.20	[−]
ρ_o(400 bar)	800 and 1000	[kg/m^3]
ρ_w(400 bar)	1000	[kg/m^3]
c_o	10^{-5}	[1/bar]
c_w	10^{-5}	[1/bar]
μ_o	10^{-3}	[Pa s]
μ_w	10^{-3}	[Pa s]
$\mathbf{v}$	8000	[m^3]
p_{cow}	0	[bar]
p_{bh}	390–415	[bar]
p (0) (top)	400	[bar]
S (0)	0.10	[−]

Note that due to the constant bottom-hole pressures in the wells, the pressure in the reservoir always stays between 390 bar and 415 bar. The initial water saturation is 0.10 throughout the reservoir.

The performance measure is NPV as defined in Eq. (16), using the values in Table 2. The goal is to maximize NPV by varying the valve settings of the 8 injectors and 4 producers over the interval [0, T]. Three different terminal times are considered: 1.5, 3.0, and 4.5 years. These reservoir flooding problems can be written as Problem 1.

The previously described reservoir model is implemented in a proprietary reservoir simulator that also comprises the required adjoint model to compute switching functions (*i.e.* gradients). The differential equations described in Section 3 are approximated using a fully-implicit scheme, with a maximum time-step size of 1/50 year (≈ 1 week).

5.2. Results

The base case comparison is a conventional water flooding strategy. Here, all valve settings are initially

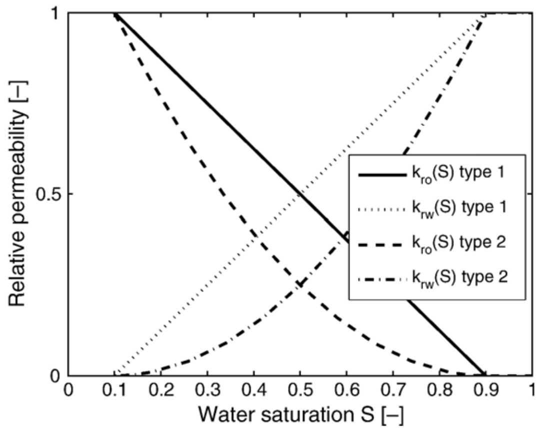

Fig. 3. Relative permeabilities for cases in Table 3.

Table 2
Values for computing NPV

Symbol	Value	Unit
r_{oil}	20	[$/bbl]
r_{prod}	5	[$/bbl]
r_{inj}	0 and 1	[$/bbl]
d	0	[1/s]
T	1.5, 3.0 and 4.5	[years]

one, but a producer valve setting is shut in (and stays shut in) when it is no longer profitable to produce from it. With r_{oil} = 20 $/bbl and r_{prod} = 5 $/bbl, this profitability threshold corresponds to a water cut of 80%.

In order to find the optimal valve settings, the conventional steepest descent method (34)–(35) is used, with u also divided into intervals of 1/50 year and initial guess $\mathbf{u}^k = 1$. At each iteration k, the step size s^k is repeatedly reduced by a factor 2 until $J(\mathbf{u}^{k+1}) \geq J(\mathbf{u}^k)$, whereupon it is increased by a factor 1.6 for the beginning of the next iteration. Initially, s^k is set to 10^{-5}.

The effects of terminal time, oil density, relative permeability, and water injection cost on the shape of the optimal solution are investigated by considering 6 numerical examples defined in Table 3, where results are also summarized.

For Case 1, the scheme indeed converges to a pure bang-bang control. We stress that this procedure could converge to a smooth solution, but does not because the optimal solution is apparently a pure bang-bang control. The optimal control for Case 1, denoted by u^*, is depicted in Fig. 4. The first order necessary optimality conditions are satisfied for u^*, as can be seen by inspection of the sign of the corresponding switching function β^*. At first sight, the strategy for the producers seems to be a reactive one. In fact this is not true: the second producer valve is shut in at a water cut of 60% — far below the profitability threshold of 80%.

From Fig. 4, it can be seen that u^* satisfies the assumptions (a)–(d) in Section 3.3, and we can therefore check second order sufficient optimality conditions. Clearly, u^* has only one switching time at $\tau^* = 1.12$ years for producer 2. Fig. 5 shows that $\frac{\partial^2 J}{\partial \tau^2}(\tau^*) < 0$. In other words, u^* really is locally optimal.

For Cases 2–6, the scheme does not converge to a bang-bang control, but to one with brief singular arcs for certain injectors. This situation is depicted for Case 2 in Figs. 6 and 7).[4]

[4] β_i^{**} (t) is almost, but not identically, zero for $t \in [1.58, 2.52]$. This is why its sign is not gray in Fig. 6.

Table 3
NPV and shape of reactive, optimal and suboptimal conrols

Case	T [yrs]	Type of relperm	r_{inj} [\$/bbl]	ρ_{o} [kg/m^3]	Type of control	Shape of control	NPV [billion \$]	Increase [%]
1	1.5	2	0	800	Reactive		1.350	
					Optimal	Bang-bang	1.365	0.8
2	3.0	2	0	800	Reactive		1.871	
					Optimal	Singular	1.934	3.4
					Suboptimal	Bang-bang	1.933	3.3
3	3.0	2	0	1000	Reactive		1.832	
					Optimal	Singular	1.893	3.3
					Suboptimal	Bang-bang	1.892	3.3
4	3.0	2	1	800	Reactive		1.736	
					Optimal	Singular	1.822	5.0
					Suboptimal	Bang-bang	1.821	4.9
5	3.0	1	0	800	Reactive		1.988	
					Optimal	Singular	2.070	4.1
					Suboptimal	Bang-bang	2.070	4.1
6	4.5	1	1	1000	Reactive		1.900	
					Optimal	Singular	2.140	12.6
					Suboptimal	Bang-bang	2.119	11.5

The improvement in NPV of the optimal control compared to the reactive control is up to 12.6% — see Table 3. The cumulative oil and water production of both strategies for $T=4.5$ years are shown in Fig. 8. Since there is no discount factor involved ($d=0$), the increase in NPV is solely due to a decrease in water production.

Improved valve settings can also be found using the alternative descent method Eq. (37), with u again divided into intervals of 1/50 year and initial guess $\mathbf{u}^k=1$. At each iteration k, the step size $\tilde{s}^k$ is repeatedly reduced by a factor 2 (and rounded off to the nearest integer) until $J(\mathbf{u}^{k+1})\geq J(\mathbf{u}^k)$, whereupon it is increased by a factor 1.6 (and rounded off to the nearest integer) for the beginning of the next iteration. Initially, $\tilde{s}^k$ is set to 30.

For Case 1, the scheme converges to the same solution as that obtained with the steepest descent method. For the other situations, however, the scheme converges to a solution that is only slightly suboptimal (meaning with

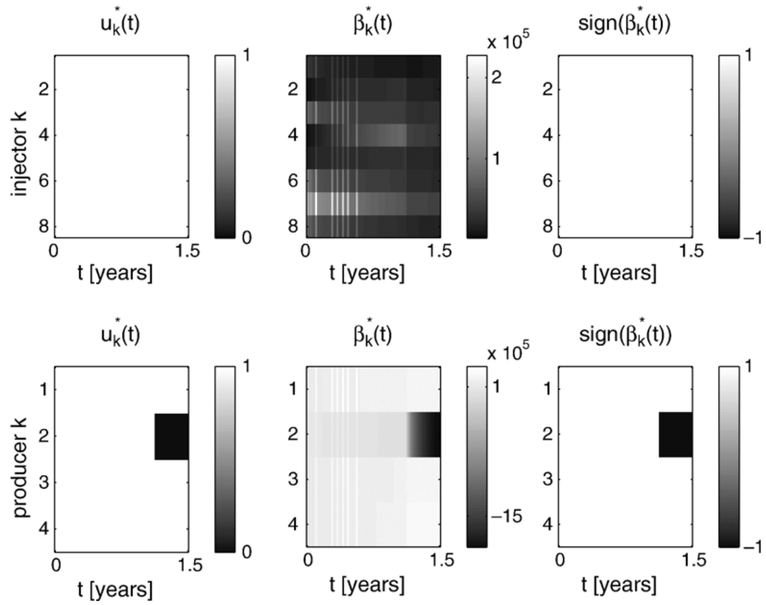

Fig. 4. Optimal valve settings u* and (sign) of the corresponding switching function β* for Case 1.

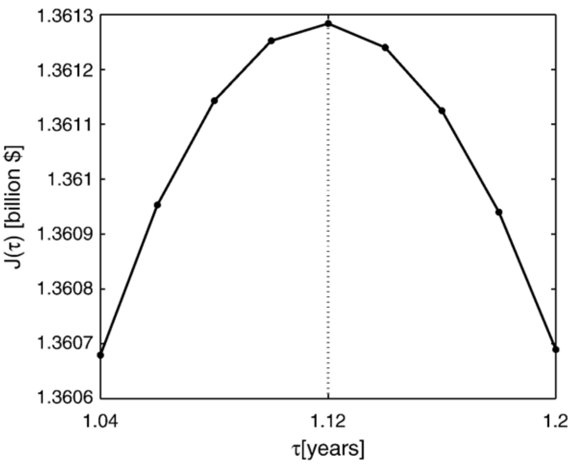

Fig. 5. NPV as a function of the switching time τ.

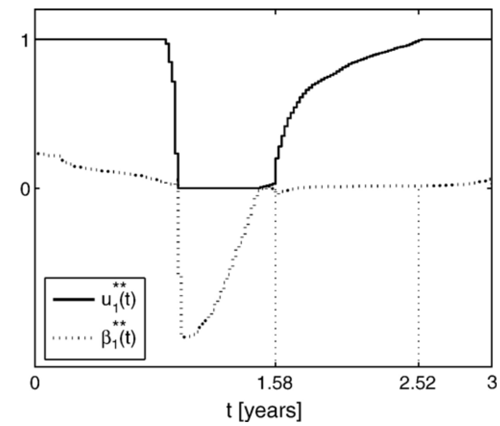

Fig. 7. Valve settings u_1^{**} and (scaled) switching function β_1^{**} of injector 1 from Fig. 6; there is a singular arc along the interval [1.58, 2.52].

only a small loss in NPV) — see Table 3. Obviously, this loss in NPV must be traded-off against the practical advantage of being able to implement the solution with simple on–off control valves.

Remarks

- Oil density does not seem to have a significant effect on the shape of the optimal solution. However, we do expect singular arcs to play a significant role in coning problems, where it is common to operate wells below the highest allowable rate.
- Water injection costs do not seem to have a significant effect on the shape of the optimal solution.
- Later terminal times generally lead to more and longer singular arcs. It would be interesting to see if this holds for problems with significant discounting in NPV.
- Problems with type 1 relative permeabilities (see Fig. 3) generally have more and longer singular arcs than those with type 2 relative permeabilities.
- For Case 1, several (very similar) solutions were found that all satisfy the necessary conditions for

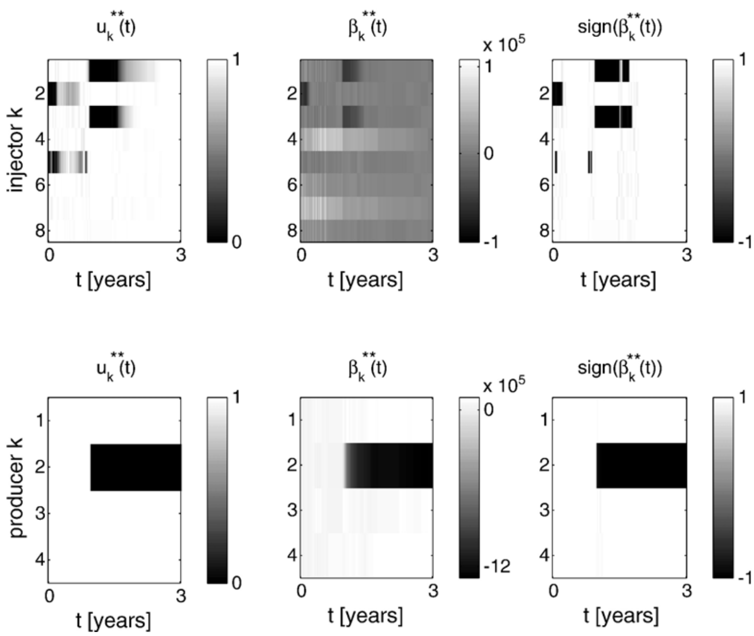

Fig. 6. Optimal valve settings u** and (sign) of the corresponding switching function β^{**} for Case 2.

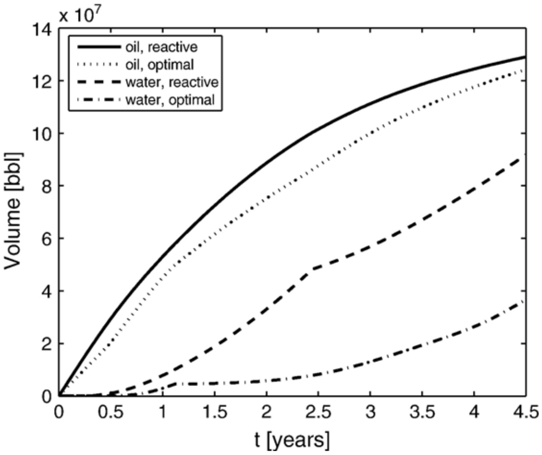

Fig. 8. Cumulative oil and water production of the reactive and optimal control for Case 6.

optimality. The one shown in Fig. 4 is the one with the highest NPV.

— There seems to be more scope for optimization in problems with later terminal times, type 1 relative permeabilities and, in particular, higher water injection costs.

6. Conclusions

Many reservoir flooding problems can be written as optimal control problems that are linear in the control. This paper shows that if the only constraints are upper and lower bounds on the control, due to their particular structure, these problems will sometimes have bang-bang optimal solutions. This is supported by a water flooding example, where for various situations the optimal solution is either bang-bang, or a bang-bang solution exists that is only slightly suboptimal. This has obvious practical implications, since bang-bang solutions can be implemented with simple on–off control valves.

Nomenclature

o, w, g	Oil, water, gas
inj, prod	Injection, production
p	Pressure
p_{bh}	Bottom-hole pressure
p_{cow}	Capillary pressure
S	Saturation
t	Time
T	Terminal time
$\nabla\cdot$	Divergence operator
∇	Gradient operator
$\bar{u}$	Superficial velocity
ϕ	Porosity
ρ	Density
c	Compressibility
k	Absolute permeability
k_{r}	Relative permeability
μ	Viscosity
q	Source/sink term
$\mathbf{v}$	Volume
$\tilde{\lambda}$	Fluid mobility
f_{w}	Fractional flow rate of water
α	Valve setting
w	Well index
N	Number of grid blocks
$\mathcal{N}$	Set of grid block indices
x	State
x_0	Initial condition
f, f_1, f_2	Nonlinear functions defining $\dot{x}$
$V, \tilde{V}, \tilde{T}$	Nonlinear functions defining f_1 and f_2
u	Control
$u_{\min}, u_{\max}$	Lower, upper bound
m	Number of controls
$\mathcal{U}$	Set of allowable controls
J	Performance measure
l, l_1, l_2, ψ	Nonlinear functions defining J
d	Discount factor
r	Revenue/cost per unit volume
λ	Adjoint
H	Hamiltonian
v	Variation of u
ε	Bound on $\mathcal{L}_1$-norm of $v-u$
o	Round-off error term
β	Switching function
n	Number of switching times
τ	Bang-bang vector of switching times
K	Number of intervals in $[0, T]$
$\mathbf{u}^k, \tilde{\mathbf{u}}^k$	Parameters defining u
$s^k, \tilde{s}^k$	Step sizes used in descent methods
Ω_1^k, Ω_2^k	Sets of indices used in descent method

Appendix A

If there is only one grid block and constant capillary pressure, we can write

$$x = [p_{\mathrm{o}}\ S_{\mathrm{w}}]^T \tag{38}$$

$$\frac{d}{dt}V(x) = \phi\frac{d}{dt}\begin{bmatrix}\rho_{\mathrm{o}}(p_{\mathrm{o}})[1-S_{\mathrm{w}}]\\ \rho_{\mathrm{w}}(p_{\mathrm{o}})S_{\mathrm{w}}\end{bmatrix}. \tag{39}$$

By defining the fluid compressibilities c_{w} and c_{o} as

$$c_{\mathrm{o}}(p_{\mathrm{o}}) = \frac{1}{\rho_{\mathrm{o}}(p_{\mathrm{o}})}\frac{d\rho_{\mathrm{o}}}{dp_{\mathrm{o}}}(p_{\mathrm{o}}) \tag{40}$$

$$c_{\mathrm{w}}(p_{\mathrm{o}}) = \frac{1}{\rho_{\mathrm{w}}(p_{\mathrm{o}})} \frac{d\rho_{\mathrm{w}}}{dp_{\mathrm{o}}}(p_{\mathrm{o}}) \tag{41}$$

we can derive that

$$\begin{aligned} \frac{d}{dt}V(x) &= \phi \begin{bmatrix} \rho_{\mathrm{o}}(p_{\mathrm{o}})(1-S_{\mathrm{w}})c_{\mathrm{o}}(p_{\mathrm{o}})\frac{dp_{\mathrm{o}}}{dt} - \rho_{\mathrm{o}}(p_{\mathrm{o}})\frac{dS_{\mathrm{w}}}{dt} \\ \rho_{\mathrm{w}}(p_{\mathrm{o}})S_{\mathrm{w}}c_{\mathrm{w}}(p_{\mathrm{o}})\frac{dp_{\mathrm{o}}}{dt} + \rho_{\mathrm{w}}(p_{\mathrm{o}})\frac{dS_{\mathrm{w}}}{dt} \end{bmatrix} \\ &= \underbrace{\phi \begin{bmatrix} \rho_{\mathrm{o}}(p_{\mathrm{o}})(1-S_{\mathrm{w}})c_{\mathrm{o}}(p_{\mathrm{o}}) & -\rho_{\mathrm{o}}(p_{\mathrm{o}}) \\ \rho_{\mathrm{w}}(p_{\mathrm{o}})S_{\mathrm{w}}c_{\mathrm{w}}(p_{\mathrm{o}}) & \rho_{\mathrm{w}}(p_{\mathrm{o}}) \end{bmatrix}}_{=:\tilde{V}(x)} \begin{bmatrix} \frac{dp_{\mathrm{o}}}{dt} \\ \frac{dS_{\mathrm{w}}}{dt} \end{bmatrix} \end{aligned} \tag{42}$$

The $\frac{d}{dt}Vx$ term in Eq. (9) can thus be written as $\tilde{V}(x)\dot{x}$. Furthermore, as long as the fluids are compressible (meaning $c_{\mathrm{w}} \neq 0$ and $c_{\mathrm{o}} \neq 0$), $\tilde{V}(x)$ is invertible. The same reasoning applies to multiple grid blocks and saturation-dependent capillary pressures.

References

Agrachev, A., Stefani, G., Zezza, P., 2002. Strong optimality for a bang-bang trajectory. SIAM J. Control Optim. 41 (4), 991–1014.

Aitokhuehi, I., Durlofsky, L.J., Artus, V., Yeten, B., Aziz, K., 2004. Optimization of advanced well type and performance. 9th European Conference on the Mathematics of Oil Recovery, Cannes.

Asheim, H., 1987. Optimal control of water drive. SPE J. (SPE 15978).

Asheim, H., 1988. Maximization of water sweep efficiency by controlling production and injection rates. SPE European Petroleum Conference (SPE 18365), London.

Athans, M., 1966. The status of optimal control theory and applications for deterministic systems. IEEE Trans. Automat. Contr. 11 (3), 580–596.

Athans, M., Falb, P.L., 1966. Optimal Control — An Introdution to the Theory and Its Applications. McGraw–Hill.

Aziz, K., Settari, A., 1979. Petroleum Reservoir Simulation. Applied Science Publishers.

Bangerth, W., Klie, H., Wheeler, M.F., Stoffa, P., Sen, M., 2006. On optimization algorithms for the reservoir oil well placement problem. Comput. Geosci. 10, 303–319.

Belghith, S.F., Lamnabhi-Lagarrigue, F., Rosset, M.M., 1986. Bang-bang solutions for a class of problems arising in thermal control. In: Reichel, D. (Ed.), Algebraic and Geometric Methods in Nonlinear Control Theory, pp. 623–632.

Bellman, R., 1956. On the "bang-bang" control problem. Q. Appl. Math. 14, 11–18.

Blakemore, N., Aris, R., 1962. Studies in optimization — v. the bang-bang control of a batch reactor. Chem. Eng. Sci. 17, 591–598.

Bressan, A., 1985. A high-order test for the optimality of bangbang controls. SIAM J. Control Optim. 23, 38–48.

Brouwer, D.R., Jansen, J.D., 2004. Dynamic optimization of waterflooding with smart wells using optimal control theory. SPE J. (SPE 78278-PA) 9 (4), 391–402.

Brouwer, D.R., Naevdal, G., Jansen, J.D., van Kruijsdijk, C.P.J.W., 2004. Improved reservoir management through optimal control and continuous model updating. SPE Annual Technical Conference and Exhibition (90149-MS), Houston.

Brouwer, D.R. (2004). Dynamic Water Flood Optimization With Smart Wells Using Optimal Control Theory. PhD thesis, Delft University of Technology.

Bryson, A.E., Ho, Y.C., 1975. Applied Optimal Control: Optimization, Estimation and Control. Hemisphere–Wiley.

Clarke, F.H., 1983. Optimization and Nonsmooth Analysis. John Wiley & Sons.

Fathi, Z., Ramirez, W.F., 1984. Optimal injection policies for enhanced recovery: part 2 — surfactant flooding. SPE J. 24 (3), 333–341.

Fathi, Z., Ramirez, W.F., 1986. Use of optimal control theory for computing optimal injection policies for enhanced oil recovery. Automatica 22 (1), 33–42.

Fathi, Z., Ramirez, W.F., 1987. Optimization of an enhanced oil recovery process with boundary controls — a large-scale non-linear maximization. Automatica 23 (3), 301–310.

Glashoff, K., Sachs, E., 1977. On theoretical aspects of the bang-bang principle. Numer. Math. 29, 93–113.

Hubbert, M.K., 1956. Darcy's law and the field equations of the flow of underground fluids. Petrol. Trans. AIME (749-G) 207, 222–239.

Jansen, J.D., Brouwer, D.R., Naevdal, G., Kruijsdijk, C.P.J.W.V., 2005. Closed-loop reservoir management. First Break 23, 43–48.

Kawski, M., 2003. High-order maximum principles. New Trends in Nonlinear Dynamics and Control. Springer–Verlag, pp. 313–326.

Kraaijevanger, J.F.B.M., Egberts, P.J.P., Valstar, J.R., Buurman, H.W., 2007. Optimal waferflood design using the adjoint method. Reservoir Simulation Symposium (SPE 105764), Houston.

Krener, A.J., 1973. The high order maximum principle. In: Reidel, D. (Ed.), Geometric Methods in System Theory, pp. 174–184.

Ledzewicz, U., Schattler, H., 2002. Optimal bang-bang controls for a two-compartment model in cancer chemotherapy. J. Optim. Theory Appl. 114 (3), 609–637.

Liu, W., Ramirez, W.F., Qi, Y.F., 1993. Optimal control of steamflooding. SPE J. (SPE 21619) 1 (2), 73–82.

Lucas, S.K., Kaya, C.Y., 2001. Switching-time computation for bang-bang control laws. IEEE American Control Conference, pp. 176–181. Arlington.

Luenberger, D.G., 1981. Introduction to Dynamic Systems: Theory, Models and Applications. John Wiley & Sons.

Maurer, H., Buskens, C., Kim, J., Kaya, C., 2005. Optimization methods for the verification of second order sufficient conditions for bang-bang controls. Optim. Control Appl. Methods 26, 129–156.

Mehos, G.J., Ramirez, W.F., 1989. Use of optimal control theory to optimize carbon dioxide miscible-flooding enhanced oil recovery. J. Pet. Sci. Eng. 2, 247–260.

Meier, L., Bryson, A.E., 1990. Efficient algorithm for time-optimal control of a two-link manipulator. J. Guid. Control Dyn. 13 (5), 859–866.

Mohler, R., 1973. Bilinear Control Processes. Academic Press.

Peaceman, D.W., 1977. Fundamentals of Numerical Reservoir Simulation. Elsevier Scientific.

Pontryagin, L.S., Boltyanskii, V.G., Gamkrelidze, R.V., Mishchenko, E.F., 1962. The Mathematical Theory of Optimal Processes. John Wiley & Sons.

Ramirez, W.F., Fathi, Z., 1984. Optimal injection policies for enhanced recovery: part 1— surfactant flooding. SPE J. 24 (3), 328–332.

Sarma, P., Aziz, K., Durlofsky, L.J., 2005. Implementation of adjoint solution for optimal control of smart wells. SPE Reservoir Simulation Symposium (SPE 92864), Houston.

Sarma, P., Chen, W.H., Durlofsky, L.J., Aziz, K., 2006. Production optimization with adjoint models under nonlinear control-state path inequality constraints. SPE Intelligent Energy Conference and Exhibition, (SPE 99959-MS), Amsterdam.

Stengel, R.F., 1986. Stochastic Optimal Control — Theory and Application. John Wiley & Sons.

Sudaryanto, B., Yortsos, Y., 2000. Optimization of fluid front dynamics in porous media using rate control 1. equal mobility fluids. Phys. Fluids 12 (7), 1656–1670.

Sudaryanto, B., Yortsos, Y., 2001. Optimization of displacements in porous media using rate control. SPE Annual Technical Conference and Exhibition (SPE 71509).

Sussmann, H., 1979. A bang-bang theorem with bounds on the number of switchings. SIAM J. Control Optim. 17 (5), 629–651.

Yeten, B., Durlofsky, L.J., Aziz, K., 2003. Optimization of nonconventional well type, location, and trajectory. SPE J. (SPE 86880-PA) 8 (3), 200–210.

Zandvliet, M.J., Jansen, J.D., Van den Hof, P.M.J., Bosgra, O.H., Kraaijevanger, J.F.B.M., 2006. Bang-bang control in reservoir flooding. 10th European Conference on the Mathematics of Oil Recovery, Amsterdam.