Computers and Chemical Engineering 35 (2011) 2227–2234

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

A perturbation approach for consistent initialization of index-1 explicit differential–algebraic equations arising from battery model simulations

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ARTICLE INFO

Article history:
Received 9 February 2010
Received in revised form 3 January 2011
Accepted 5 January 2011
Available online 12 January 2011

Keywords:
DAE
Initialization
Consistent initial condition
Perturbation approach
Index-1 DAEs

ABSTRACT

Estimation of consistent initial conditions is very crucial for the successful solution of differential–algebraic equation (DAE) systems that arise in many fields of science and engineering. In this paper, an efficient perturbation approach for initialization of DAE systems of index-1 is proposed and implemented for DAE models governing batteries. In addition, different existing solvers are compared for consistent initialization of DAE systems. The proposed approach does not necessarily require a nonlinear solver for initialization and builds on the applicability and usability of robust and efficient explicit, linearly implicit and semi-implicit integrators in time. Three different problems are presented wherein the proposed approach is observed to work for a wider range of inconsistent initial conditions compared to other existing generally used routines. It is also observed that the present approach is computationally efficient compared to the other existing approaches in a given environment.

1. Introduction

Dynamic physical processes arise in many areas of engineering, science and economics, and are usually modeled using ordinary differential equations (ODEs) or partial differential equations (PDEs). However, some of the states in these physical processes are constrained, and such states are governed by algebraic equations and the resulting mathematical model contains ODEs/PDEs coupled with nonlinear algebraic equations (Kunkel & Mehermann, 2000). Numerical solution of DAE systems is more difficult as compared to ODE models due to the existence of linear and non-linear algebraic equations and due to discontinuities in the algebraic variables over the independent variable space. A DAE system in general is characterized by its index, which is defined as the number of differentiations required to convert a DAE system into an ODE system. Higher the index of the system, less reliable the solutions are with classical numerical methods. DAE systems of index greater than 2 are in general difficult to solve and is still an active area of research.

In modeling of various chemical and electrochemical processes, DAE models of index-1 are commonly encountered, in particular during simulation of batteries at different operating conditions wherein simulation of continuous charge/discharge curves involve state detections. For a system of DAEs, some solution approaches involve differentiation of the algebraic equations to obtain ODEs for algebraic variables. Differentiation process may impose additional constraints and add stiffness. Depending on the algorithm chosen to solve a DAE model, the original constraints may not be satisfied due to the error introduced by the numerical computation of the differentiated constraints (Garcia, 2000). Another difficulty that arises while solving a DAE model is the lack of consistent initial conditions. While solving a DAE model, it is crucial to use consistent initial conditions for both the differential and the algebraic variables. However, in many modeling situations, consistent initial conditions may not be directly available for all the variables. This is especially true for batteries where state of charge and state of health change with the number of cycles and state events may happen at different points in the performance curves. Consequently, many good solvers fail to solve DAE models resulting from simulation of battery models (Wu & White, 2001).

Estimation of consistent initial conditions is a challenging step and very crucial for the successful solution of DAE models. Several methods have been proposed for the estimation of consistent initial conditions in the literature. Sincovec, Erisman, Yip, and Epton (1981) suggested integration of the DAE systems of index-n with implicit Euler method. After at least n steps, the solution trajectory will be reached, and the computed value of algebraic variables will be a set of consistent initial conditions. A variation of this method was used in the DASSL solver (Brenan et al., 1989) for the calculation of initial derivatives of algebraic variables for a given set of consistent values. Kröner et al. (1992) made further improvements in integration step size selection and error control of the initializa-

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doi:10.1016/j.compchemeng.2011.01.003

Nomenclature

a_i	specific surface area of electrode i ($i = p, n$), m^2/m^3
c	electrolyte concentration, mol/m^3
c_0	initial electrolyte concentration, mol/m^3
$c_{s,i}$	concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3
$c_{s,i,0}$	initial concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3
$c_{s,i,max}$	maximum concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3
D	electrolyte diffusion coefficient, m^2/s
$D_{s,i}$	lithium ion diffusion coefficient in the intercalation particle of electrode i ($i = p, n$), m^2/s
F	Faraday's constant, C/mol
I	applied current density, A/cm^2
i_1	solid phase current density, A/m^2
i_2	solution phase current density, A/m^2
j_s	solvent reduction current density, $mol/m^2 s$
j_i	wall flux of Li^+ on the intercalation particle of electrode i ($i = p, n$), mol/m^2 s
k_i	intercalation/deintercalation reaction rate constant of electrode i ($i = p, n$), $mol/(mol/m^3)^{1.5}$
l_i	thickness of region i ($i = p, s, n$), m
n	negative electrode
p	positive electrode
r	radial coordinate, m
R	universal gas constant, J/(mol K)
s	separator
t^+	Li^+ transference number in the electrolyte
T	absolute temperature, K
x	spatial coordinate, m
ε_i	porosity of region i ($i = p, s, n$)
κ	ionic conductivity of the electrolyte, S/m
$\kappa_{eff,i}$	effective ionic conductivity of the electrolyte in region i ($i = p, s, n$), S/m
ρ_s	density of the solvent reduction product film, g/m^3
σ_i	electronic conductivity of the solid phase of electrode i ($i = p, n$), S/m
$\sigma_{eff,i}$	effective electronic conductivity of the solid phase of electrode i ($i = p, n$), S/m
Φ_1	solid phase potential, V
Φ_2	electrolyte phase potential, V

tion algorithm used in the DASSL routine. Gear (1971) presented an algorithm where he used explicit Euler formulation for a DAE system and then Newton's method was used for the corrections. If the correction step does not meet the convergence criteria, then the Jacobian is reevaluated. The author suggested that the algorithm will be useful for a DAE system with multiple solutions for the algebraic variables, provided the multiple solutions remain distinct within the error criteria.

Pantelides (1988) proposed a method based on a graph-theoretical approach for finding the minimal set of equations in order to obtain a semi-explicit index-1 DAE system. Unger, Kröner, and Marquardt (1995) implemented a slightly different version of Pantelides' algorithm based on the structural analysis of the sparsity patterns of the Jacobian matrix of the system. Kröner, Marquardt, and Gilles (1997) suggested the use of restrictive damping strategies if a DAE system is encountered with steep gradients. Vieira and Biscaia Jr. (2001) proposed an initialization technique which is based on the approximation of dynamic response of a system with a discontinuous perturbation of a similar system. Mrziglod (1987) based his algorithm on detailed decomposition of the DAE system; however this approach requires knowledge of the analytical expressions for differentiations. A pure numerical approach was proposed by Leimkuhler, Petzold, and Gear (1991) for a DAE system of index-n. The authors construct the consistency equations with total differentials for the DAE system with time up to an order n. The resulting set of equations was solved using the least square approach. Existence and uniqueness of solution was proved by the authors for a DAE system with linear coefficients. Reissig, Boche, and Barton (2002) proposed an initialization approach based on the Laplace transform for the time invariant linear DAEs. In this approach, consistent initial conditions of DAE systems were estimated using mapping functions. They also mentioned that for every DAE system there exists a unique family of mapping functions. Reis (2007) considered the consistent initialization differential–algebraic systems on infinite-dimensional Hilbert spaces based on a decoupling form where he formulated sufficient criteria for an initial value being consistent with a given inhomogeneity. The initial value thus had to fulfill not only algebraic relations being hidden in the system but also the (hidden) boundary constraints that come. He also formulated perturbation results for consistently initialized systems. Lamour and Mazzia (2009) combined the results concerning the solvability of DAEs with properly stated leading terms with an appropriate method for the approximation of the derivative, and proposed an algorithm that provides the necessary data to formulate the initial conditions. The authors stated that this method works at least for nonlinear DAEs up to index 3. Estévez Schwarz (2009) defined and analyzed DAEs in nonlinear Hessenberg form of arbitrary high order with regard to consistent initialization. For this class of DAEs, he proposed that the hidden constraints can be systematically described and the consistent initialization can be determined through step-by-step solving of linear sub-problems.

Efforts have also been made for estimation of consistent initial conditions using optimization techniques. Vieira and Biscaia Jr. (2000) compared various initialization techniques and proposed a method based on the optimization strategy. In their approach, they optimized a set of equations consisting of consistency equations, additional constraints and hidden constraints estimated using differentiations. The authors suggested that hybrid optimization methods are more appropriate for the estimation of consistent initial conditions. Gopal and Biegler (1999) used a sequential linear programming approach for estimation of initial conditions with and without discontinuities.

Several solvers are available for solutions of DAE models such as LSODI (Nuclear Energy Agency website, 2010), LIMEX (Deuflhard, Hairer, & Zugck, 1987), DASSL (Brenan et al., 1989), and RADAU5 (Hairer & Wanner, 1991). Recently, many easy to use ODE solvers (ode15s, ode15i, etc.) from MATLAB® (Mathworks website, 2010), "NDsolve" from MATHEMATICA® (Wolfram website, 2010), and "dsolve" from MAPLE® (Maplesoft website, 2010) are available to solve non-stiff, stiff and moderately stiff DAE models of index-1. A more recent software package is JACOBIAN® (Numerica Technology website, 2010), a general purpose modeling and optimization package, which features numerical algorithms for systems of hybrid discrete and continuous DAEs. Its initialization procedure uses Newton–Raphson technique. It also handles sparse Jacobians of DAE systems through sparse direct methods, which is often more convenient than preconditioned Krylov methods.

Many of these solvers fail to solve the DAE models for batteries with inconsistent initial conditions but on the other hand work reasonably well with consistent initial conditions (for both dependent variable and its derivative). Wu and White (2001) presented an initialization subroutine (DAEIS) which was based on a nonlinear equation solver. They showed that the range for inconsistent initial conditions was broader for the DAEIS subroutine than with some

of the readily available solvers such as LSODI, LIMEX, and DASSL for DAE models.

In spite of these recent advancements, many of these DAE solvers and initialization routines fail due to the convergence problem of Newton iteration and the singular/ill-conditioned Jacobian matrix resulting from a small integration step. When convergence criteria of Newton iterations are not satisfied, these solvers reduce integration step size to a smaller value. This may be a good approach for a DAE system with nearly consistent initial conditions, but may not be useful with inconsistent initial conditions that are far off from the consistent initial conditions. Due to a very small step size, Jacobian matrix becomes singular, resulting in failures of the DAE solvers. Therefore, the available DAE solvers with initialization routines might fail with inconsistent initial conditions (Wu & White, 2001).

In this paper, an efficient approach for finding consistent initial conditions for a DAE system is presented. This approach is based on the singular perturbation method and the use of efficient ODE solvers in a dummy variable. We estimated consistent initial conditions for DAE systems arising from the battery models and the results are presented in Section 3. To our knowledge, singular perturbation technique has been attempted to only solve DAEs directly (Garcia, 2000) (by perturbing the entire system including the ODEs and algebraic equations). However, this results in forcing the perturbed dynamics of the ODE variables and algebraic variables to the dynamics of the original system. In addition, for using explicit solvers to integrate the resulting ODEs with time-variant mass-matrix, there is a need to invert Jacobian matrices for the full system as opposed to the algebraic equations alone. The proposed approach in this paper uses the perturbation approach only to find the consistent initial conditions, which once obtained can be used to solve the original set of DAEs with readily available solvers.

2. Efficient approach for consistent initial conditions for DAE systems

Consider a physical process represented by the following DAE system

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(t, \boldsymbol{y}, \boldsymbol{z}) \tag{1a}$$

$$\boldsymbol{0} = \boldsymbol{g}(t, \boldsymbol{y}, \boldsymbol{z}) \tag{1b}$$

where we assume that $\boldsymbol{f}$ and $\boldsymbol{g}$ are differentiable (at least once), and $\boldsymbol{y} \in \Re^n$, $\boldsymbol{z} \in \Re^m$ are the differential and algebraic variables of the system respectively. This set of equations results from modeling of some physical process, or discretization of spatial variables of partial differential equations (PDEs). To find consistent initial conditions for the algebraic variables ($\boldsymbol{z}$), initial conditions for differential variables are substituted in Eq. (1b) to have

$$\boldsymbol{g}(t_0, \boldsymbol{y}_0, \boldsymbol{z}) = 0 \tag{2}$$

At time $t = 0$, $\boldsymbol{z}(0)$ has to be found that satisfies

$$\boldsymbol{g}(t_0, \boldsymbol{y}_0, \boldsymbol{z}_0) = 0 \tag{3}$$

Many initialization solvers including DAEIS use nonlinear equation solving subroutine to solve $\boldsymbol{g}(t_0) = 0$ (the functional dependence of $\boldsymbol{g}$ on $\boldsymbol{y}$ and $\boldsymbol{z}$ is dropped henceforth for simplicity), which may not converge easily and nonlinear solvers require high computational effort. Instead, if we assume a perturbation parameter ε, which is a very small constant such that

$$\boldsymbol{g}(t) = \lim_{\varepsilon \to 0} \boldsymbol{g}(t + \varepsilon) = 0 \tag{4}$$

Then algebraic part of the given DAE model (Eq. (1b)) at time $t = t + \varepsilon$ can be written as

$$\boldsymbol{g}(t + \varepsilon) = 0 \tag{5}$$

Expanding $\boldsymbol{g}(t + \varepsilon) = 0$ using the Taylor series expansion, we have

$$\boldsymbol{g}(t) + \varepsilon \frac{d\boldsymbol{g}(t)}{dt} + O(\varepsilon^2) = 0 \tag{6}$$

In Eq. (6), t is an arbitrary dummy variable and can be replaced with τ as,

$$\boldsymbol{g}(\tau) + \varepsilon \frac{d\boldsymbol{g}(\tau)}{d\tau} = 0 \tag{7}$$

Eq. (7) can be written in terms of the partial derivatives as

$$\boldsymbol{g} + \varepsilon \left[\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \tau} + \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \tau} + \frac{\partial \boldsymbol{g}}{\partial \tau} \right] = 0 \tag{8}$$

Equation (8) can be simplified as

$$\boldsymbol{g} + \varepsilon \left[\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}} \boldsymbol{f} + \boldsymbol{J}_{alge} \frac{\partial \boldsymbol{z}}{\partial \tau} + \frac{\partial \boldsymbol{g}}{\partial \tau} \right] = 0 \tag{9}$$

which can be written in compact form after substituting the initial value for differential variables as

$$-\varepsilon \times \boldsymbol{J}_{alge} \times \left[\frac{\partial \boldsymbol{z}}{\partial \tau} \right] = \boldsymbol{F}_{alge}(\tau, \boldsymbol{z}) \tag{10}$$

where

$$\boldsymbol{F}_{alge} = \boldsymbol{g} + \varepsilon \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}} \boldsymbol{f} + \varepsilon \frac{\partial \boldsymbol{g}}{\partial \tau}$$

$$\boldsymbol{J}_{alge} = \begin{bmatrix} \frac{\partial g_1}{\partial z_1} & \cdots & \frac{\partial g_1}{\partial z_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial g_m}{\partial z_1} & \cdots & \frac{\partial g_m}{\partial z_m} \end{bmatrix} \tag{11}$$

where m is the number of algebraic variables. As $\varepsilon \to 0$, and when the steady state is reached, $\boldsymbol{g} = 0$ will be satisfied in Eq. (7). The crucial factor in Eq. (10) is the Jacobian matrix. The accuracy of the convergence of this ODE system with time depends on the nature of the problem, ε, accuracy of the Jacobian evaluation, and the tolerance required.

Finally, the resulting equation is in the form of a dummy differential variable τ, which can be solved using the available ODE solvers until the steady state of all the algebraic variables or the convergence criterion in $\boldsymbol{g}$ is met.

At steady state, we have $\boldsymbol{F}_{alge} = \boldsymbol{0}$, which means

$$\boldsymbol{g} + \varepsilon \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}} \boldsymbol{f} + \varepsilon \frac{\partial \boldsymbol{g}}{\partial \tau} = 0 \tag{12}$$

By choosing ε to be very low and waiting till a steady state is reached, we have,

$$\boldsymbol{F}_{alge} \cong \boldsymbol{g}(t_0) = 0 \tag{13}$$

The validity of Eq. (7) or (10) can be easily verified for linear systems of equations.

It can be proved (at least for linear systems) that the solution of $\boldsymbol{F}_{alge}$ will reach the steady state (consistent initial condition) as time goes to infinity. The dynamics of the solution depends on ε, and the difference between the initial guess and the consistent solution. For very low values of ε in Eq. (10), numerical solvers might face difficulties. The wider range of the proposed approach reported in this paper can be primarily contributed to the ability of the approach to reach the steady state irrespective of the initial conditions.

The resulting system of equations after applying the proposed perturbation approach (Eq. (10)) is in the form of an ODE that can be solved using the plethora of good ODE solvers that are available in the literature. The ODE solvers can be chosen to be implicit, semi-implicit, or explicit and not requiring a nonlinear solver at any point in the dummy variable τ (including intermediate time steps). To use explicit solvers, Eq. (10) can be rewritten as

$$\boldsymbol{J}_{alge}\frac{d\boldsymbol{z}}{d\tau} = -\frac{\boldsymbol{F}_{alge}(\tau, \boldsymbol{z})}{\varepsilon} \tag{14}$$

However, the left hand side of Eq. (14) needs to be factorized and then directly used in explicit solvers such as LSODI. (Alternatively one can invert $\boldsymbol{J}_{alge}$ matrix and use explicit solvers, however, inversion is not recommended for large systems.) This approach provides the advantage of faster simulation time with a wide range of inconsistent initial conditions for the DAE system. The system of DAE can now be solved with the available solvers using the consistent initial conditions obtained by the above approach.

The proposed approach differs from Davidenko's approach (Davidenko, 1953) for the solution of nonlinear algebraic equations; which is given by

$$\boldsymbol{J}\frac{d\boldsymbol{z}}{d\tau} = -\boldsymbol{g} \tag{15}$$

where $\boldsymbol{J}$ and $\boldsymbol{g}$ are the Jacobian matrix and function vector of the algebraic system. Davidenko's approach does not include partial derivatives of $\boldsymbol{g}$ with respect to $\boldsymbol{y}$ and τ. Since $\boldsymbol{g}$ is originally a function of $\boldsymbol{y}$, $\boldsymbol{z}$, and τ, Taylor series expansion with partial derivatives used in this paper is more accurate. When the partial derivatives with respect to $\boldsymbol{y}$ and τ are zero for $\boldsymbol{g}$, the proposed approach reduces to Davidenko's approach for $\varepsilon = 1$. It can be concluded that the proposed approach provides a wider range of validity compared to Davidenko's approach.

The applicability of the proposed approach is evaluated by solving some of the difficult problems of different dimensions reported in the battery domain. Particularly, we have evaluated the efficacy of the above approach with a simple numerical example of a DAE system (a DAE system of dimension 2 with 1 algebraic equation and 1 ODE) followed by the problem described by Wu and White (2001) (a DAE system of dimension 2 with 1 algebraic equation, 1 ODE) for a Ni based battery, the reformulated model of lithium-ion battery (Subramanian, Boovaragavan, Ramadesigan, & Arabandi, 2009) (a DAE system of dimension 27 with 15 algebraic equations and 12 ODEs) and the finite difference descretized model of lithium-ion battery proposed by Newman and his group (Doyle, Fuller, & Newman, 1993) (a DAE system of dimension 300 with 181 algebraic equations and 119 ODEs). A schematic of the proposed initialization approach is given in Fig. 1.

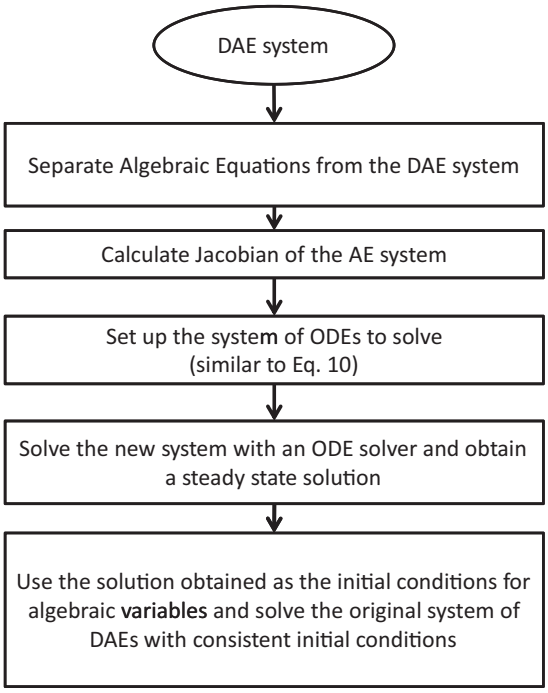

Fig. 1. Schematic of the proposed initialization method for simulation of index-1 DAE systems.

3. Results and discussion

3.1. DAE system of dimension 2 (1 algebraic equation and 1 ODE)

Consider a simple DAE system as described below where z is a differential variable and y is an algebraic variable. The latter examples in this paper illustrate the importance of the proposed approach in a better manner compared to this particular problem. However, this is a much simpler problem and is presented only to illustrate the procedure of solving a system of DAEs with the proposed initialization approach.

$$\frac{dz}{dt} = -2z + y^2 \tag{16}$$

$$-100\ln y + 2z = 5 \tag{17}$$

The initial value of the differential variable can be set as

$$z(0) = 2 \tag{18}$$

Step by step solution of the above equations using the proposed method is discussed below.

Eq. (17) is satisfied when the initial condition for the algebraic variable y is $\exp(-0.01)$, and only a very few solvers work when values other than this is given as initial condition. The above equations are not solvable directly in majority of solvers that come built in with mathematical packages like Maple®, Matlab®, etc. when the initial value of y is given a value other than $\exp(-0.01)$. To increase the range of initial values we use the proposed method as follows. To estimate the exact initial condition, the proposed approach involves applying Eq. (10) as

$$\varepsilon\left(-\frac{100(dy/dt)}{y} + 2\frac{dz}{dt}\right) = 100\ln(y) - 2z(0) + 5 \tag{19}$$

where ε is the perturbation parameter. Substituting Eq. (16) and the initial condition of $z(0)$ in the above equation we get

$$\varepsilon\left(-\frac{100(dy/dt)}{y} - 8 + 2(y)^2\right) = 100\ln(y) + 1 \tag{20}$$

The above equation can be solved using any available ODE solver with different initial guesses and carefully choosing the value of the perturbation parameter, to obtain a steady state solution for y, which will be the consistent initial condition and can be used for solving the original set of DAEs and obtain the desired solution.

Table 1 gives the range of values of initial conditions for y that can be given for successful simulation of the above equations using various solvers. Table 1 lists the range of initial values of y that work with the built in initialization approach of each solver and also the range of values with the proposed approach. It can be seen that, a few recent solvers like JACOBIAN® have a wider range with the built in approach, however the other solvers still fail for a value far away from the consistent initial value. Table 1 also gives an idea of how sensitive the range of initial conditions is for different values of ε, the choice of which must be carefully made since too small

Table 1
Working range of inconsistent initial values and ε for the problem in Section 3.1 for various solvers.

Solver	With fixed $z(0) = 2.0$, range for $y(0)$
DASKR	$0.15 \le y(0) \le 1.82$
DASSL	$0.890 \le y(0) \le 1.090$
DASSL (Davidenko initialization)	$1.E{-}16 \le y(0) \le 690{,}030$
JACOBIAN	$1.E{-}300 \le y(0) \le 1.E300$
Proposed approach (JACOBIAN)	$1.E{-}300 \le y(0) \le 15{,}800$, $\varepsilon = 1.E{-}7$ $1.E{-}300 \le y(0) \le 5.E6$, $\varepsilon = 1.E{-}12$ $1.E{-}300 \le y(0) \le 5.E8$, $\varepsilon = 1.E{-}16$ $1.E{-}300 \le y(0) \le 1.E300$, $\varepsilon \le 1.E{-}29$
Proposed approach (DASKR)	$1.E{-}40 \le y(0) \le 70{,}000$, $\varepsilon = 1.E{-}7$ $1.E{-}40 \le y(0) \le 2.9E7$, $\varepsilon = 1.E{-}12$ $1.E{-}40 \le y(0) \le 180$, $\varepsilon = 1.E{-}14$ No convergence, $\varepsilon = 1.E{-}16$
Proposed approach (DASSL)	$1.E{-}16 \le y(0) \le 12{,}510$, $\varepsilon = 1.E{-}6$ $1.E{-}16 \le y(0) \le 14$, $\varepsilon = 1.E{-}7$ $1.E{-}16 \le y(0) \le 3.7$, $\varepsilon = 1.E{-}10$ No convergence, $\varepsilon \le 1.3E{-}11$
Consistent value	$y(0) = 0.9900498390197754$ Found by DASKR and JACOBIAN This is close to proposed method results if $\varepsilon = 1.E{-}7$

values of ε would make the system unstable/stiff and unsolvable. The following examples illustrate the importance of the proposed approach for use with battery models.

3.2. DAE system of dimension 2 (1 algebraic equation and 1 ODE)

The following DAE system arises while modeling the galvanostatic charge/open-circuit/discharge processes of a thin film nickel hydroxide electrode. This system is of dimension 2, in which y_1 and y_2 are mole fractions of nickel hydroxide and potential difference at the solid liquid interface respectively.

$$\frac{\rho V}{W}\frac{dy_1}{dt} = \frac{j_1}{F}$$

$$j_1 + j_2 - i_{app} = 0$$

where

$$j_1 = i_{01}\begin{bmatrix} 2(1-y_1)\exp\left(\dfrac{0.5F}{RT}\right)(y_2 - \phi_{eq,1}) \\ -2y_1\exp\left(-\dfrac{0.5F}{RT}\right)(y_2 - \phi_{eq,1}) \end{bmatrix}$$
$$j_2 = i_{02}\begin{bmatrix} \exp\left(\dfrac{F}{RT}\right)(y_2 - \phi_{eq,2}) \\ -\exp\left(-\dfrac{F}{RT}\right)(y_2 - \phi_{eq,2}) \end{bmatrix} \quad (21)$$

The parameter values are given in Table 2. The units of system variables and parameters are omitted here for simplicity. The consistent initial values of dependent variables in Eq. (21) are not easily available from the modeling information. For a discharged nickel electrode, the initial value of the differential and algebraic variables are estimated as

$$y_1(0) = 0.05$$
$$y_2(0) = 0.38 \quad (22)$$

which are not consistent values with respect to Eq. (21).

Many available DAE solvers failed to solve this system of equation with the initial guess values given by Eq. (22) (Wu & White, 2001). In addition, many DAE initialization subroutines and solvers failed to solve this system of equations over a wide range of inconsistent initial conditions. We have used eight available solvers or initialization subroutines (given in Table 3) for either solving this equation with the initial guess given by Eq. (22) or estimating the consistent initial condition.

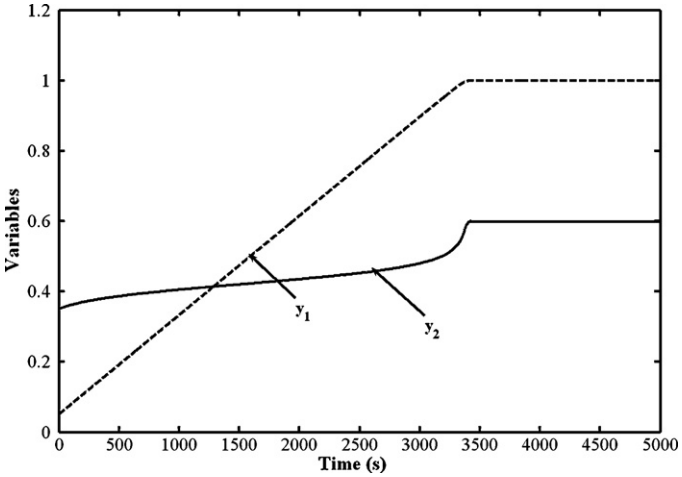

Fig. 2. Simulation of a DAE system governing the galvanostatic charge/open-circuit/discharge processes of a thin film nickel hydroxide electrode given by Wu and White (2001), with consistent initial conditions.

For the approach described in this paper, Eq. (21) can be cast into the reduced system of equation for estimating the consistent initial condition according to Eq. (10) as

$$\begin{aligned}
&\varepsilon\begin{pmatrix} -0.0002\,e^{19.46229155y_2 - 8.174162450} \\ -0.0002\,e^{-19.46229155y_2 + 8.174162450} \end{pmatrix} \\
&\times\begin{pmatrix} 0.005651477584(1-y_1(0))\,e^{19.46229155y_2 - 8.174162450} \\ -0.005651477584y_1(0)\,e^{-19.46229155y_2 + 8.174162450} \end{pmatrix} \\
&+\varepsilon\begin{pmatrix} 0.003892458310(1-y_1(0))\,e^{19.46229155y_2 - 8.174162450} \\ +0.003892458310y_1(0)\,e^{-19.46229155y_2 + 8.174162450} \\ +0.000000003892458310\,e^{38.92458310y_2 - 11.79414868} \\ +0.000000003892458310\,e^{-38.92458310y_2 + 11.79414868} \end{pmatrix} \quad (23) \\
&\times\frac{dy_2}{d\tau} \\
&= -0.0002(1-y_1(0))\,e^{19.46229155y_2 - 8.174162450} \\
&+ 0.0002y_1(0)\,e^{-19.46229155y_2 + 8.174162450} \\
&- 0.0000000001\,e^{38.92458310y_2 - 11.79414868} \\
&+ 0.0000000001\,e^{-38.92458310y_2 + 11.79414868} + 0.00001
\end{aligned}$$

where ε and y_1 are the perturbation parameter and differential variable respectively. Corresponding solution obtained from our approach is plotted in Fig. 2. Comparison of performance of various solvers and initialization subroutines along with the method described above are given in Table 3. Table 3 shows the convergence range of the algebraic variable (initial guess) with different available DAE solvers and the proposed approach. As y_1 is the differential variable, we only estimated the range for the algebraic variable y_2. The error messages obtained from various solvers are given as

- *LIMEX: MORE THAN JRMAX = 20 STEP-SIZE REDUCTIONS DUE TO EXTRAPOLATION TABLEAU*
- *RADAU5: MATRIX IS REPEATEDLY SINGULAR*
- *DASSL: THE CORRECTOR FAILED TO CONVERGE REPEATEDLY OR WITH ABS(H) = HMIN*
- *MATLAB: NEEDS A BETTER GUESS y_0 FOR CONSISTENT INITIAL CONDITIONS*
- *MATHEMATICA: UNABLE TO FIND INITIAL CONDITIONS THAT SATISFY THE RESIDUAL FUNCTION WITHIN SPECIFIED TOLERANCES*
- *JACOBIAN: INITIALIZATION FAILED, SIMULATION FAILED*

Table 2
Parameter used for the simulation of nickel electrode (Section 3.2).

Parameters	Value	Parameters	Value
F (Faraday's constant), C/mol	96,487	V (volume), m^3	1×10^{-5}
R (universal gas constant), J/(mol K)	8.314	i_{01} (exchange current density), A/cm^2	1×10^{-4}
T (temperature), K	298.15	i_{02} (exchange current density), A/cm^2	1×10^{-10}
$\phi_{eq,1}$ (equilibrium potential), V	0.420	i_{app} (applied current density), A/cm^2	1×10^{-5}
$\phi_{eq,2}$ (equilibrium potential), V	0.303	ρ (density), g/cm^3	3.4
W (mass of active material), g	92.7		

Table 3
Working range of the inconsistent initial values for various solvers.

Solver	With fixed $y_1(0) = 0.05$, range of $y_2(0)$
LIMEX	$0.318 \le y_2(0) \le 0.377$
RADAU5	$0.348 \le y_2(0) \le 0.352$
DASSL	$0.321 \le y_2(0) \le 0.370$
DASSL (Davidenko initialization)	$-0.74 \le y_2(0) \le 1.54$
MATLAB® (ode15s)	$-0.31 \le y_2(0) \le 0.93$
MAPLE® (dsolve, numeric)	Failure for any value other than consistent initial condition
MATHEMATICA® (NDSolve)	$-0.27 \le y_2(0) \le 1.04$
DAEIS	$-0.974 \le y_2(0) \le 1.663$
JACOBIAN®	$-10.5 \le y_2(0) \le -9.5,\ -6.5 \le y_2(0) \le -5.5,\ -4.0 \le y_2(0) \le -2.85,\ -2.0 \le y_2(0) \le 1.515$
Proposed approach (MAPLE®)	$-10 \le y_2(0) \le 10$
Proposed approach (JACOBIAN®)	$-17.1 \le y_2(0) \le 17.7$
Proposed approach (DASSL)	$-16.3 \le y_2(0) \le 16.45$
Proposed approach (approximate, MAPLE®)	$-0.67 \le y_2(0) \le 1.5$
Consistent value	$y_2(0) = 0.35024$

It is observed that the proposed perturbation based initialization approach has a broader range for inconsistent initial conditions as compared to the other available solvers and initialization subroutines (see Fig. 3 and Table 3). We have also solved this system of equations with an approximate perturbation approach. Here, approximate perturbation approach means substituting the initial values of the dependent variables in the left hand side of Eq. (23) for the Jacobian matrix. This results in the following equation which can be solved using explicit solvers

$$\begin{aligned} &0.1620939380\varepsilon + 0.3297276483\varepsilon\frac{dy_2}{d\tau} \\ &= -0.000190\, e^{19.46229155y_2 - 8.174162450} \\ &+0.000010\, e^{-19.46229155y_2 + 8.174162450} \\ &-0.0000000001\, e^{38.92458310y_2 - 11.79414868} \\ &+0.0000000001\, e^{-38.92458310y_2 + 11.79414868} + 0.00001 \end{aligned} \quad (24)$$

It was found that the solution procedure is computationally efficient (because of the simplicity of the equation) but the domain/range of the inconsistent initial condition reduces significantly. It is also observed that with JACOBIAN® solver, the range of proposed approach is much wider than with the solvers in MAPLE® environment. Hence, the selection of solvers for numerical simulation of the resulting ODE system has an effect on the range of validity of the proposed approach.

Fig. 4 shows the effect of perturbation parameter on the speed of convergence of the algebraic variable. This figure is plotted using the initial guess of 5 for the algebraic variable y_2 in Eq. (23) and changing the value of the perturbation parameter. It is observed that with decreasing value of the perturbation parameter ε, the speed of convergence increases (i.e. the system reaches the steady state quickly). Note that decreasing the values of perturbation parameter improves the accuracy and the speed of convergence. However, the stiffness of the equations increases with decreasing

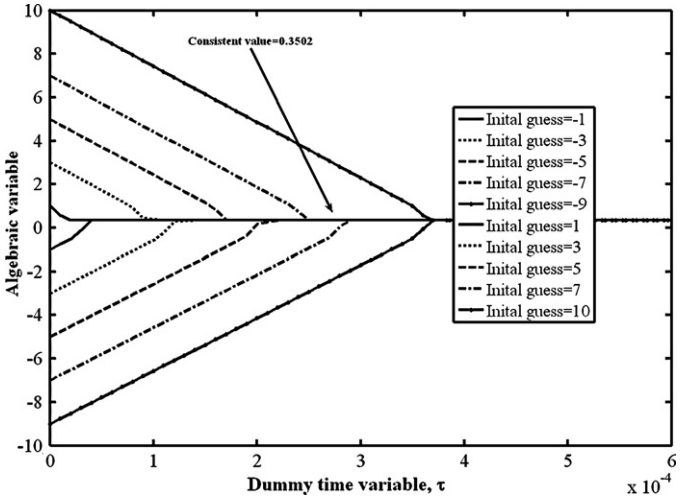

Fig. 3. Wider range of inconsistent initial conditions using the proposed approach for the simulation of a DAE system governing the galvanostatic charge/open-circuit/discharge processes of a thin film nickel hydroxide electrode given by Wu and White (2001).

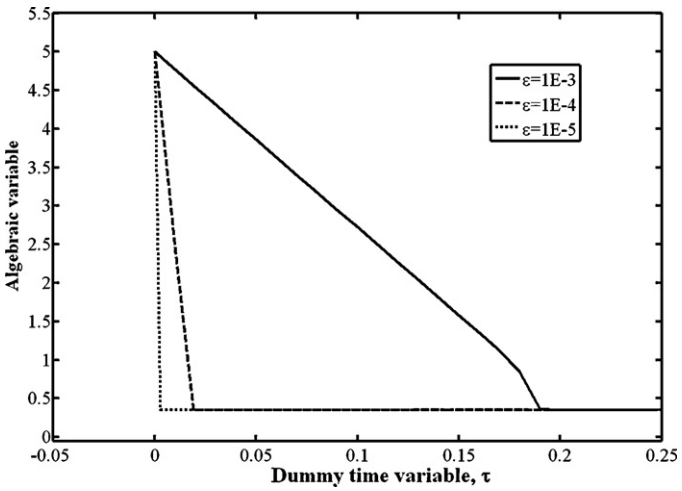

Fig. 4. Effect of perturbation parameter, ε on the speed of convergence (attaining steady state) with the proposed approach with inconsistent initial conditions for the algebraic variable.

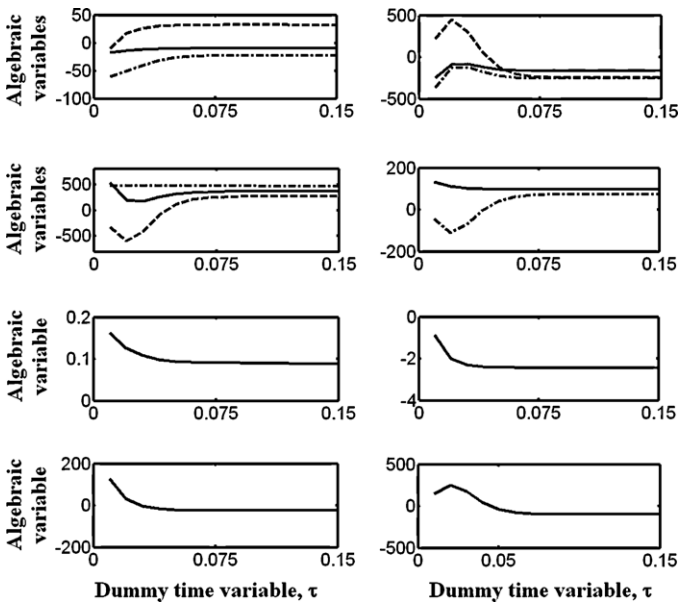

Fig. 5. Steady state (consistent initial conditions) profiles of the algebraic variables of the reformulated model for a lithium-ion battery using the proposed approach.

the perturbation parameter below a certain value. Our experience suggests that for values of the perturbation parameter lesser than 10^{-9}, many solvers become too slow and computationally inefficient when the steady state is expected at $\tau \simeq 1$.

3.3. DAE system of dimension 27 (15 algebraic equations and 12 ODEs)

The reformulated model used in this work is derived from the first-principles porous electrode-based electrochemical engineering model of lithium-ion battery (Subramanian et al., 2009). This model consists of 27 DAEs out of which 12 are ODEs and 15 are algebraic equations. In battery modeling scenario, the consistent initial conditions are unknown to the modeler and hence these types of DAEs are difficult to solve even with very good DAE solvers. We tried to solve this system of equations in many solvers available within MAPLE®, MATLAB®, and with DASSL, and observed the failure of the initialization subroutine of these solvers for the set of parameters we used. For brevity, we are not providing details of the modeling equations in this paper, but interested readers can find more details elsewhere (Subramanian et al., 2009).

The reformulated model is cast as described in Section 2 and the perturbation approach is used to find the consistent initial conditions. It is observed that the perturbation approach estimates consistent initial conditions for all the algebraic variables efficiently (see Fig. 5). Fig. 5 shows the plot of algebraic variables attaining steady state based on the above mentioned approach for the reformulated model of lithium-ion battery. It is also observed that the "FSOLVE" subroutine in MAPLE® (which uses analytic Jacobian) often encounters failure while solving this system of equations with inconsistent initial conditions. The total CPU time taken by "FSOLVE" is approximately 41 s in comparison with 0.360 s using the approach described in this paper (written in Maple® environment) in a PC with a 2.6 GHz dual core processor and 2GB of RAM. Note that the CPU time reported depends on the environment and the solvers used. The object of this paper is to illustrate the robustness of the proposed approach to obtain consistent initial conditions in an efficient manner for a DAE system.

To compare the proposed approach with other solvers, we used JACOBIAN® solver for the initialization of reformulated model. It was observed that the computational efficiency of the proposed approach for the reformulated model is comparable with JACOBIAN®. Nevertheless, the range of inconsistent set of initial conditions is broader as compared with that of the built-in initialization routine in JACOBIAN®. For a set of inconsistent initial conditions, we multiplied the consistent set of initial conditions with a constant number. It is found that proposed approach works with the constant varying in the range of −3.5 to 8.5 whereas JACOBIAN® works for a range of 0.766–2.719. It is also observed that compared to other existing solvers (LIMEX, RADAU5, DASSL, NDSOLVE, ode15s, and dsolve), JACOBIAN® solver works for a wider range of inconsistent initial conditions.

3.4. DAE system of dimension 300 (with 181 algebraic equations and 119 ODEs)

Another example used for testing the efficacy of the proposed approach is a pseudo 2 dimensional lithium-ion battery model developed by Newman (Doyle et al., 1993). This model consists of a porous electrode, a separator, and a current collector. The independent variables for the lithium-ion battery model are the two spatial variables x, r, and time variable t. It should be noted that the variations in r direction is approximated using a parabolic profile model (Gu, Wang, & Liaw, 1998; Subramanian, Diwakar, & Tapriyal, 2005; Wang, Gu, & Liaw, 1998). The governing equations for all these variables are given in Table 4 and the explanations for variables and other quantities and expressions are available elsewhere (Subramanian et al., 2005). A related model (BVP) in x was initialized using a modified multiple shooting technique earlier (Boovaragavan & Subramanian, 2007; Keller, 1968).

Lithium-ion battery model given in Table 3 discretized with 25, 25, and 15 grid points in the two electrodes and the separator respectively using finite difference method, resulted in 300 DAEs. This set of finite difference equations was cast as described in Section 2 and the consistent initial conditions were evaluated. It is observed that the proposed perturbation approach estimates consistent initial conditions for all the algebraic variables efficiently. It is also observed that the "FSOLVE" subroutine in MAPLE® encounters failure while solving this system of equations when the grid points are increased beyond 6, 6 and 3 in the two electrodes and the separator respectively.

The above model was successfully run for $N = 5$, 10, 20, 30, etc. It is interesting to note that the battery model converges for N as low as 10 node points, but solvers like DASSL/DASKR fails without initialization at $N = 10$, 15, 20 or 30 node points. However, if we use very high node points, say $N = 100$ or 200 node points, DASSL can initialize by tweaking the tolerances by trial and error. The proposed method works at different values of N, and is faster than the inbuilt initialization methods of solvers when using very high node points. The use of initialization developed here helps us simulate battery models even at lower to middle number of node points thereby reducing the simulation time required by a large amount.

4. Limitations

It is observed that the proposed approach has the following limitations

(1) The proposed approach is valid only for explicit DAEs of index-1.
(2) The efficiency of this approach depends on the value of perturbation parameter. It is found that, lower the value of the perturbation parameter, in general lower than 10^{-6}; stiffer will be the set of equations to solve (Eq. (10)) using ODE solvers.

Table 4
Governing equations for DAE of dimension 300, for describing galvanostatic discharge of a lithium-ion battery (Doyle et al., 1993).

Region	Eq. no.	Governing equations	Boundary conditions
Positive electrode	1	$\varepsilon_p \frac{\partial c}{\partial t} = D_{eff,p} \frac{\partial^2 c}{\partial x^2} + a_p(1-t_+)j_p$	$-D_{eff,p} \frac{\partial c}{\partial x}\Big\|_{x=0} = 0$ and $-D_{eff,p} \frac{\partial c}{\partial x}\Big\|_{x=l_p,-} = -D_{eff,s} \frac{\partial c}{\partial x}\Big\|_{x=l_p,+}$
		initial condition $c\|_{t=0} = c_0$	
	2	$-\sigma_{eff,p} \frac{\partial \Phi_1}{\partial x} - \kappa_{eff,p} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{eff,p}RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x} = I$	$-\kappa_{eff,p} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=0} = 0$ and $-\kappa_{eff,p} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p,-} = -\kappa_{eff,s} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p,+}$
	3	$\sigma_{eff,p} \frac{\partial^2 \Phi_1}{\partial x^2} = a_p F j_p$	$\frac{\partial \Phi_1}{\partial x}\Big\|_{x=0} = -\frac{I}{\sigma_{eff,p}}$ and $\Phi_1 = 4.2$
	4	$\frac{d}{dt} c_s^{ave} + 3\frac{j_p}{R_p} = 0$ and $\frac{D_{s,p}}{R_p}(c_s^{surf} - c_s^{ave}) = -\frac{j_p}{5}$	$c_s^{ave}\Big\|_{t=0} = c_{s,\max,p}$
Separator	5	$\varepsilon_s \frac{\partial c}{\partial t} = D_{eff,s} \frac{\partial^2 c}{\partial x^2}$	$-D_{eff,p} \frac{\partial c}{\partial x}\Big\|_{x=l_p,-} = -D_{eff,s} \frac{\partial c}{\partial x}\Big\|_{x=l_p,+}$ and $-D_{eff,s} \frac{\partial c}{\partial x}\Big\|_{x=l_p+l_s,-} = -D_{eff,n} \frac{\partial c}{\partial x}\Big\|_{x=l_p+l_s,+}$
	6	$I = -\kappa_{eff,s} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{eff,s}RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x}$	$-\kappa_{eff,p} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p,-} = -\kappa_{eff,s} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p,+}$ and $-\kappa_{eff,s} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p+l_s,-} = -\kappa_{eff,n} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p+l_s,+}$
	7	$\varepsilon_n \frac{\partial c}{\partial t} = D_{eff,n} \frac{\partial^2 c}{\partial x^2} + a_n(1-t_+)j_n$	$-D_{eff,s} \frac{\partial c}{\partial x}\Big\|_{x=l_p+l_s,-} = -D_{eff,n} \frac{\partial c}{\partial x}\Big\|_{x=l_p+l_s,+}$ and $-D_{eff,n} \frac{\partial c}{\partial x}\Big\|_{x=l_p+l_s+l_n} = 0$
Negative electrode		initial condition $c\|_{t=0} = c_0$	
	8	$-\sigma_{eff,n} \frac{\partial \Phi_1}{\partial x} - \kappa_{eff,n} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{eff,n}RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x} = I$	$-\kappa_{eff,s} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p+l_s,-} = -\kappa_{eff,n} \frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p+l_s,+}$ and $\frac{\partial \Phi_2}{\partial x}\Big\|_{x=l_p+l_s+l_n} = 0$
	9	$\sigma_{eff,n} \frac{\partial^2 \Phi_1}{\partial x^2} = a_n F j_n$	$-\sigma_{eff,n} \frac{\partial \Phi_1}{\partial x}\Big\|_{x=l_p+l_s} = 0$ and $\frac{\partial \Phi_1}{\partial x}\Big\|_{x=l_p+l_s+l_n} = -\frac{I}{\sigma_{eff,n}}$
	10	$\frac{d}{dt} c_s^{ave} + 3\frac{j_n}{R_n} = 0$ and $\frac{D_{s,n}}{R_n}(c_s^{surf} - c_s^{ave}) = -\frac{j_n}{5}$	$c_s^{ave}\Big\|_{t=0} = c_{s,\max,n}$

5. Conclusions

The proposed approach is based on an iteration free solver in a dummy variable form with a wider range of validity compared to iteration based direct nonlinear solvers. This initialization approach can be used when initialization failure is encountered with many of the available DAE solvers. The examples demonstrated in this paper show that the proposed approach can solve a DAE system of large dimensions efficiently. It is observed that there is a trade-off between the ranges of inconsistent initial conditions and the computational time for simulation using this approach. The initialization approach developed and described in this paper was found to be efficient for explicit DAEs of index-1.

Acknowledgements

The authors are thankful for the partial financial support of this work by the National Science Foundation under contract number CBET-0828002 and CBET-1008692, International Center for Advanced Renewable Energy and Sustainability at Washington University in St. Louis (I-CARES) and the U.S. government.

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