steel research international

Modelling and Simulation of the Melting Process in Electric Arc Furnaces—Influence of Numerical Solution Methods

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Increasing demands on the steel market are leading to introduction of many technological innovations regarding the electric arc furnaces (EAFs). The area with significant potential is also advanced computer support, based on mathematical models estimating the process values which are not continuously measured, such as chemical compositions and temperatures of the steel, slag and gas. To achieve optimal process control using EAF models, two crucial characteristics of the later are required, i.e. sufficient accuracy and calculation speed, both affected by selection of the modelling approach and ordinary differential equation (ODE) solving method. The aim of this paper is to investigate the estimation accuracy and calculation speed of an EAF model, evaluated by three solving methods, i.e. fixed step Euler, variable step Runge-Kutta and Backward Differentiation Formula (BDF). The results are showing that the selection of the ODE solver has an enormous effect on simulation outcome. All three methods proved to be appropriate to obtain the estimated process values; however, achieving a desired level of precision leads to significant deviations in computational speeds. Thus, when aiming for optimal model based EAF control, proper selection of the ODE solver is as important as the modelling approach, but too often neglected.

1. Introduction

The field of EAF modelling has expanded greatly in the last two decades and has become a tool, which is given considerable attention as an EAF operation support system. The models that have been developed can be classified in different categories according to their complexity, purpose and accuracy. They extend from the simplest,[1] describing only the basic, necessary processes, to more enhanced ones,[2–4] including more mechanisms and leading to more accurate results, to the most comprehensive configurations,[5–8] consisting of all major phenomena in the EAF, providing the most accurate estimations of the process values. In an EAF modelling literature review by Turkdogan[9] it can be seen that dynamic models have the edge over static calculations when it comes to their use for either process monitoring, optimisation or control, since static models are more focused on offline statistical studies and are usually not implemented for online calculation purposes. When building a dynamic process model, the dynamics of the modelled process are usually described by ordinary differential equations. In order to solve the ODEs numerically, which is the normal case in simulation, different ODE solving methods were developed up to now. The selection of proper ODE solver is one of the aspects that is closely related to the modelling and simulation in general, but is too often given insufficient attention.

It is known that most of the EAFs are still operated based on operator's experience and not on the actual conditions in the EAF (stage of melting, temperatures and compositions) due to the nature of the process (high temperatures and currents). Such operation of the EAF leads to sub optimal results and consequently to lower steel yield and quality and to higher energy and material consumptions, i.e. to higher operational costs. In order to optimise the EAF process, a better insight to the actual conditions in the EAF should be presented to the operator, by either extended process measurements or by estimation of the unmeasured process

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DOI: 10.1002/srin.201500141

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values using complex process models. In this manner, approximate values of the crucial process variables, e.g. steel temperature and composition, are accessible to the operator, leading to more optimal action or decision in a given moment. In order to accurately simulate the conditions in an EAF and to present the estimation results to the operator in real time or perhaps even include an optimisation procedure, two requirements have to be met, i.e. sufficient model complexity and short enough computation time. The latter is related to all, model size, model complexity (ordinary or partial differential equations, algebraic equations etc.) and the ODE solving method. Since the model size and complexity usually cannot be changed in order to ensure sufficient accuracy, the solving method is the crucial part of the system, which significantly influences the computational speed. Moreover, the process' dynamics represented by its time constants also play an important role when solving the ODEs, as the following rule applies: the faster dynamics, i.e. short time constants, the smaller integration steps are needed for proper ODE solving. In the case of an EAF modelling, the dynamics range from very fast, i.e. some of the chemical reactions, electrical relations etc.; to very slow, i.e. heat transfers, melting etc., which represents the so called stiffness of the system, which can also be an issue for the ODE solver. For this reason a comprehensive study on the selection of the integration method for EAF process simulation has been performed, focusing on both process value estimation accuracy and computational speed for online use of the process models incorporated for different purposes, i.e. process monitoring, optimisation or control.[10,11] In this manner, the effects of three different ODE solvers are presented and compared, using a comprehensive EAF process model as a basis for calculations and three different solving methods, i.e. fixed step Euler, variable step Runge-Kutta and BDF methods.[12,13] The first ones are two of the most common methods in each category (fixed/variable step), and the third method is a special solver for stiff ODEs. For the fixed step Euler method, step sizes between 0.25 s to 0.0001 s are investigated and their influence to computational speed and accuracy for bath temperature prediction is compared to the variable step Runge-Kutta method and numerical differentiation formulas (NDF), here particularly the BDF method.

2. EAF Model

2.1. EAF Model Description

The EAF model used to perform this research presents a comprehensive combination of all crucial processes occurring during the EAF steel recycling. The models were developed in accordance with fundamental physical laws by means of first order differential equations and were tested and validated on EAF operational measurements.[5–7,10] The selected approach has its advantages and drawbacks when compared to other possibilities (e.g. fuzzy or neural network approaches, support vector machines etc.); however, the possibility to use the developed models with as many EAF designs as possible was the main aim of the development and for this reason the models are based on fundamental mathematical/physical approaches.[9] The validation of the model showed high estimation accuracy for measured average process values and satisfactory computational speed for the needs of simulation.[6,7] The achieved results for the endpoint steel temperature of 1958–K ± 10.5 K were close to the average measured temperature of 1961 K ± 11.6 K. However, whether the model shall be used as a basis for online process optimisation, its evaluation speed needs to be increased significantly. The model used in this study is schematically presented in **Figure 1**. The presented model implements mathematical equations of all main physical processes appearing during the steel recycling process, i.e. thermal (including radiation), chemical and mass transfer. As presented, the overall model is designed of several modules, each representing a set of equations describing particular physical phenomena in the EAF (energy distribution, chemical reaction, mass calculations, heat transfer etc.). Due to the complexity of the modelled processes and in order to simplify the obtained models, the EAF layout is divided into several zones (solid steel, liquid steel, solid slag, liquid slag, gas, roof and walls), assuming homogeneity and equal physical characteristics of each zone. The characteristics of each sub model are briefly explained in the following.

The heat transfer model is characterised by the following:

1. 1st order ODEs are used to calculate the temperatures of the zones and are based on energy input/output balances,
2. heat transfers are calculated for each zone from: arcs, burners, chemical reactions, volatile material oxidation, electrode oxidation and other zones,
3. heat losses are calculated due to cooling of the furnace, off-gas extraction, steel and slag enthalpy,

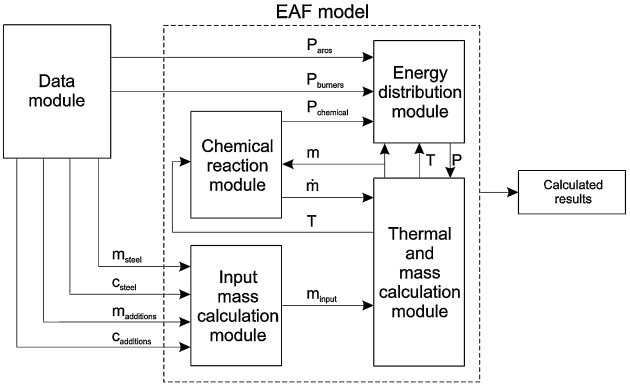

Figure 1. Schematic presentation of the EAF model used in this study.

4. calculation of the geometry supported (view-factor based) radiative heat exchange,
5. calculation of temperature dependent burner efficiency and continuous transitions between the zones (geometry supported).

The mass transfer model is characterised by the following:

1. 1st order ODEs are used to calculate the mass transfers between the zones and are based on zone temperatures and energy input/output balances,
2. elements and compounds which are used in each zone in the calculations are:
   - steel zone: Fe, C, Si, Cr, Mn,
   - slag zone: FeO, SiO_2, MnO, Cr_2O_3, CaO, MgO, Al_2O_3,
   - gas zone: N_2, O_2, CO, CO_2, CH_4,
3. consideration of reversible dynamics (cooling and solidification),
4. calculation of the mass transfers due to: melting, charging and slag addition, oxy-fuel burners, O_2 lancing, C injection and chemical reactions.

The chemical model is characterised by the following:

1. implementation of the main chemical reactions appearing in the steel melting process (oxidation of Fe, Si, C, CO, Mn, Cr; reduction of FeO, SiO_2, MnO, Cr_2O_3),
2. 1st order ODEs are used to calculate the rates of change of elements/compounds based on molar equilibria with reaction equilibria constants dependent on molar composition of the zone,
3. calculation of chemical energy exchange due to exothermic and endothermic reactions,
4. calculation of the foamy slag height, based on slag density/viscosity/surface tension and superficial gas velocity (CO) including slag decay,
5. calculation of online and endpoint steel, slag and gas compositions and relative pressure.

In the first stage of development the presented EAF model was implemented with the fixed step Euler method. For further developments and the related increase in complexity it was re-implemented in a manner that allows the use of all MATLAB R2014a integrated ODE solving methods.

2.2. New EAF Model Implementation and Comparability of Results

Due to the re-implementation, several model modifications were required to ensure a robust and stable simulation. Sudden changes through if-else conditions were removed and replaced by continuous control algorithms. These were realised by adding modified hyperbolic tangent functions with a more or less steep curve shape to switch between 'on' and 'off' resp. one and zero. Also the mode of operation had to be slightly adjusted as well as the calculation of the melting geometry to avoid sudden changes and to realise progresses without any steps. All in all, these modifications lead to small deviations in the simulation results between the old fixed step Euler method and the new implementation, but enables the usage of all current and future MATLAB R2014a integrated ODE solver or a combination of them. As a consequence, the simulation results achieved with both implementations are not directly comparable regarding the question, which solution method is the more accurate one. Instead, the results of the Euler method implementation with different decreasing time step sizes are compared among themselves as well as the MATLAB integrated ODE methods Runge-Kutta(ode45) and the BDF(ode15s) are also compared with each other.

3. Numerical Solution Methods for ODEs

Great efforts are made to model the physical processes in an EAF most precisely to predict important process variables with maximum precision. As a consequence of the relatively long simulated process time of at least 30 minutes up to more than 60 minutes for one melting period (tap to tap), the choice of the numerical solution method can influence the simulation results enormously, but is sometimes not considered in detail. The literature on solution algorithms used in EAF modelling and simulation is sparse. Even though lots of numerical EAF models can be found in literature, the focus is on the results achieved without referring to the solution method.

In case of simple model implementations using basic fixed step size methods, a conflict between accuracy and computation time arises. In order to achieve fast results, larger step sizes have to be chosen which are leading to bigger deviations in the results. When process models are applied for research or optimisation calculations, the computation time is not critical and smaller time steps can be chosen to achieve accurate results, but taking into account numerical limitations. To avoid the conflict between the simulation time and the accuracy, ODE solution methods with variable time step sizes can be applied to solve the initial value problem of the EAF model.

By realising the new implementation it turned out that the described EAF model is a stiff system of ODEs. It means that there are some components of the solution decay, which are varying much more rapidly than others. Under these circumstances, the explicit numerical methods have to take small step sizes to obtain satisfactory results. As a result, the Runge-Kutta calculation described below is still precise, but would take a long computation time. As there is no unique definition of stiffness in literature, complex ODE systems are identified to be stiff according to their behaviour.

The presented EAF model consists of 52 ODEs, describing heat and mass transfers as well as pressure change and mass changes through chemical reactions which are described in earlier publications.[6,7] The latter ODEs are changing quickly to reach equilibrium while heat and mass transfer are more or less fixed, i.e. stiff. The numerical solution methods applied for the simulation of the EAF model are shortly described below. The description gives only a short overview as there are more methods available to solve ODEs.

3.1. Fixed Step Size Euler Method

A simple, robust and frequently used method to solve initial value problems is the explicit Euler method. This method uses a self-chosen constant time increment $h > 0$ to calculate time following function values y_{n+1} according to the Equation 1, 2 and 3.[14]

$$\dot{y} = f(t, y) \qquad y(t_0) = y_0 \tag{1}$$

$$t_n = t_0 + nh \qquad n = 0, 1, 2, \ldots \tag{2}$$

$$y_{n+1} = y_n + hf(t_n, y_n) \quad n = 0, 1, 2, \ldots \tag{3}$$

The accuracy of the method depends on the change of $f(t_n,y_n)$ and the selected time step size h, which influences the resulting error proportional. The smaller the selected step size, the more accurate the result but the longer the computation time. The great advantage of the method is its robustness and the simple programming via loop calculations and therefore it was used in the first stage of development of the EAF model. The possibility of choosing bigger time steps for a fast simulation to check the plausibility and stability was accepted in contrast to the disadvantage of long simulation time for smaller time step sizes to reach high accuracy. In addition, the optimal time step size for a given accuracy cannot be calculated and thus creates a conflict of interest between accuracy and computational speed. Other Euler methods like the implicit Euler method (also known as backward Euler method) or modified Euler method are not investigated, as these methods have the same disadvantage of a self-chosen step size and are not provided by MATLAB R2014a as a standard ODE solver.

3.2. Variable Step Size Runge-Kutta Method

As a common one step solver, the explicit Runge-Kutta(4,5) formula obtains its error through a comparison of a fourth order with a fifth order Runge-Kutta calculation and reduces its step size h if necessary to achieve the specified tolerance (Dormand-Prince method).[12,14,15] The calculation rule for a fourth order Runge-Kutta method to calculate following function values y_{n+1} for step size $h > 0$ is described with **Equation 4** to **10**.

$$\dot{y} = f(t, y) \qquad y(t_0) = y_0 \tag{4}$$

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{5}$$

$$t_{n+1} = t_n + h \tag{6}$$

$$k_1 = f(t_n, y_n) \tag{7}$$

$$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{1}{2}k_1 h) \tag{8}$$

$$k_3 = f(t_n + \frac{h}{2}, y_n + \frac{1}{2}k_2 h) \tag{9}$$

$$k_4 = f(t_n + h, y_n + k_3 h) \tag{10}$$

In MATLAB R2014a, this ODE method is called ode45 and is recommended as the best function to apply as a first try for most problems with medium to high accuracy. The Runge-Kutta method is also used to solve the EAF model from Ghobara, which is based on the EAF model from MacRosty and Swartz.[3,16] For further investigation of accuracy and speed of the simulation, the ode45 is used as the reference solution for highest precision.

3.3. Variable Step Size BDF/NDF Method

When a differential problem is stiff, Runge-Kutta(ode45) fails or is very inefficient, or when solving a differential algebraic problem, it is recommended to use multi-step BDF/NDF solver. This implicit solver is based on numerical differentiation formulas, and is capable to use backward differentiation formulas which are also known as Gear's method.[13] The unknown value y_{n+1} is thereby calculated through a polynomial approximation, where the derivative of the polynomial satisfies the differential equation in point t_{n+1}. The general calculation rule to calculate following function values y_{n+1} for step size $h > 0$ is described with **Equation 11** and **12**.

$$\dot{y} = f(t, y) \qquad y(t_0) = y_0 \tag{11}$$

$$y'(t_{n+1}) = \frac{1}{h}\sum_{j=0}^{k} a_j y_{n+1-j} = f(t_{n+1}, y_{n+1}) \tag{12}$$

The coefficients a_j are calculated through derivation of the interpolation polynomial and the initial values y_1 to y_{k-1} are generated via single step methods. The BDF method

(MATLAB function ode15s) computes following process values with a variable order k by achieving low to medium accuracy and takes less computation time in each step for solving stiff implicit equations than most other numerical solution method provided by MATLAB R2014a.[17]

4. Results and Discussion

In this section, the simulation results for different solution methods are compared in terms of accuracy and speed. In particular, the bath temperature and the net heat flow of the solid scrap and the liquid melt phase are investigated by using the old and the new model implementation. In terms of the bath temperature, highest accuracy is achieved when the average measured steel bath temperature of 1961 K is reached as the final simulation result, according to the validation within the first publication of the model.[6,7] For the fixed step Euler method, step sizes between 0.25 s to 0.0001 s are investigated. The limits were selected in a way that for larger step sizes it wouldn't be possible to obtain any results due to a lack of stability and for smaller step sizes; the amount of data wouldn't longer be manageable with standard computer capacity. For the MATLAB ODE methods, the step sizes are calculated by the calculation mechanism itself. The boundary conditions for the simulations are the same as described in the first publication of the model.[6,7] The whole melting process of 85 t of scrap, divided into three baskets, corresponds to a simulated process time of 2700 s. The charging of the second and third scrap basket takes place at 900 s and 1500 s as can be seen in the results.

4.1. Simulation Run Times

Before discussing the results obtained, the simulation run times are compared first. Therefore, **Table 1** shows the different durations for the investigated step sizes with the Euler method compared to the durations of the Runge-Kutta(ode45) and NDF/BDF(ode15s) methods. For large time steps, the Euler method provides quick results due to a small number of iterations. For decreasing time step sizes, the duration increases inversely proportional in consequence of the increased number of calculation loops.

The investigated variable time step solvers are resulting in completely different simulation run times. While the Runge-Kutta(ode45) method needs around two hours to simulate the whole process, the NDF/BDF(ode15s) needs only one minute. As described before, this is attributable to the stiffness of the ODE system. The mechanism of Runge-Kutta cannot increase the time step and reaches an average step size of about 0.003 s while the ode15s calculation reaches an average time step size of about 1.2 s for the investigated model. The ode15s is much faster than the ode45 mechanism. For further comparison, the influence of the step sizes on the accuracy is discussed in the following sections.

step size [s]	Euler method [s]	Runge-Kutta(ode45) [s]	NDF/BDF(ode15s) [s]
0.25	5		
0.1	12		
0.01	113	7178	61
0.001	1133		
0.0001	12143		

Table 1. Simulation run times for the investigated numerical solution methods

4.2. Bath Temperature

Figure 2 and **Figure 3** are showing the results for the bath temperature calculation. In both figures, the bath temperature starts at 1809 K and temperature drops are visible after the charging process of cold scrap. At the end of the process, the temperature of the melt increases to reach tapping temperature. Here, the big differences in the results for the calculation with the Euler method and different step sizes are obvious in Figure 2. For increasing time step sizes, the deviations are increasing, especially for long simulated process times. For big time steps, sudden

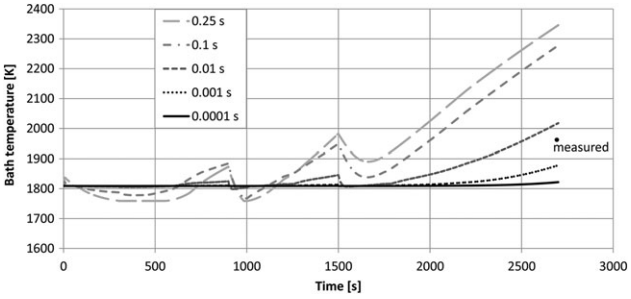

Figure 2. Bath temperature calculated with the Euler method.

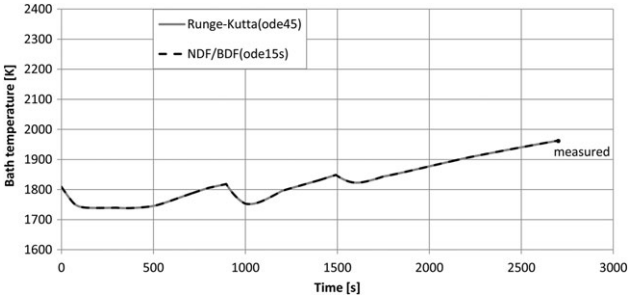

Figure 3. Bath temperature for Runge-Kutta(ode45) and NDF/BDF(ode15s).

changes of process variables are recognised in the simulation with a time delay or are even disregarded. Then smaller deviations are summing up and the calculation error growths.

For smaller time steps, the differences between the calculations are decreasing and the behaviour of the bath temperature seems to be constant with a small increase at the end of the process due to overheating. The average measured steel bath temperature of 1961 K is not reached with the used time steps and a most suitable time step would be between 0.001 s and 0.01 s. For the inaccuracy with small time steps it is assumed that the performance is attributable to numerical inconsistencies within the single loop implementation. First, the temperature change rate and a temporarily new bath temperature are computed. Second, the mixing temperature of the liquid melt at the temporarily bath temperature with the new melted scrap at melting point is computed. Due to the small time step, the change of the bath temperature is numerically very small and close to the numerical precision of MATLAB R2014a which is nearly 1e-17. This leads to rounding errors so that the proportion of the melted scrap leads to a stabilisation around the bath temperature for very small time step sizes.

In contrast to the Euler implementation, the two variable time step implementations are showing nearly the same results for the bath temperature calculation with negligible differences and both are reaching the average measured steel bath temperature. The temperature drop after charging cold scrap as well as the temperature increase at the end of the process by overheating is visible. The differences within the computed step sizes between the ode45 and ode15s mechanisms are not visible. The ode15s uses small step sizes were necessary and increases the step size were possible.

As described in section 2.2, the results between the variable step size methods and the Euler method are not directly comparable, as small adjustments in the new MATLAB implementation were necessary. Nevertheless, the simulation with the variable step solvers are reaching the final bath temperature reliably whereas the simulation with the Euler method reaches different bath temperatures dependent on the chosen time step size. As a result, the correct step size for the Euler method cannot be easily selected in advance to the simulation and consequently, a time step size optimisation for the model is necessary or the time step can be optimised in a way to compensate modelling inaccuracies.

4.3. Net Heat Flow to Scrap and Melting Phase

The heat flows to the liquid melt phase and the scrap phase are relevant to determine the melt rate and the temperature change rate of the corresponding phases. For the simulation with the Euler method, **Figure 4** and **Figure 5** show differences in the results for different time step sizes

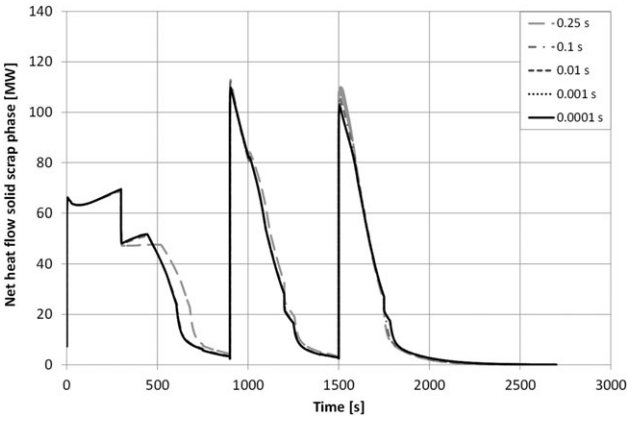

Figure 4. Net heat flow to solid scrap calculated with the Euler method.

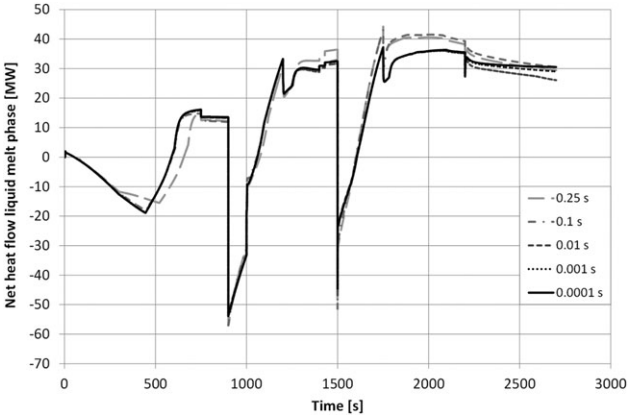

Figure 5. Net heat flow to liquid melt calculated with the Euler method.

as it is already noticeable in the results for the bath temperature calculation. For the biggest step size of 0.25 s, the time delay compared to the calculations with smaller step sizes is visible, especially when melting the first two baskets. At the end of the simulation, when melting the third basket, the deviations between the different step sizes are the biggest of up to 7 MW in the heat flow to the liquid melt phase. For a decreasing time step size, the differences between the simulation results for small time step sizes are also decreasing. As a consequence, an increase in accuracy can be assumed for small time steps, as the simulation results are less dependent on the step size. But, as described in section 4.2, the numerical precision of the simulation software has to be considered as rounding errors are possible.

The results for both variable time step implementations, Runge-Kutta and NDF/BDF, are nearly the same with negligible differences and are shown in **Figure 6** and **Figure 7**. The NDF/BDF mechanism provides the

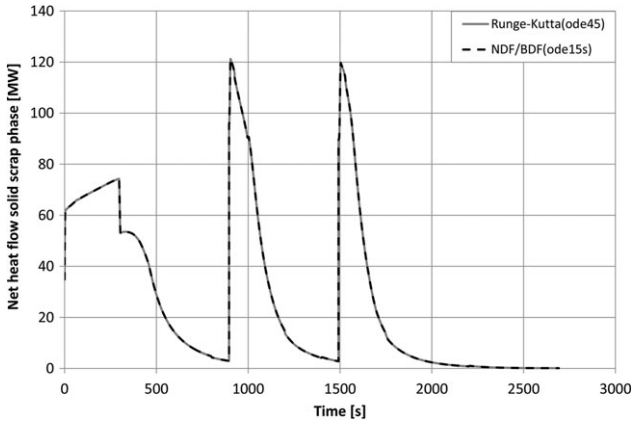

Figure 6. Net heat flow to solid scrap for Runge--Kutta(ode45) and NDF/BDF(ode15s).

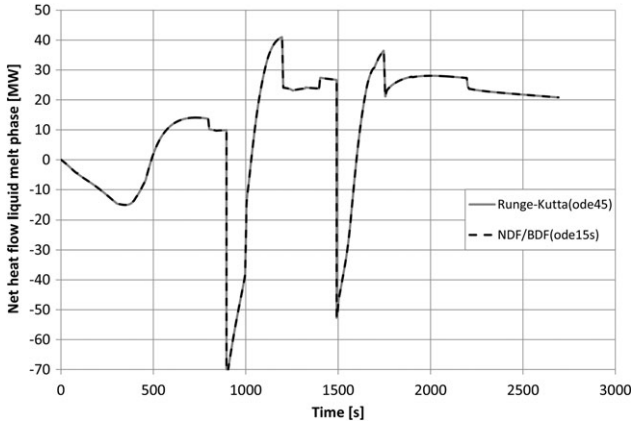

Figure 7. Net heat flow to liquid melt for Runge--Kutta(ode45) and NDF/BDF(ode15s).

simulation results much faster than the Runge-Kutta method. As described in section 3.2, Runge-Kutta is suggested as the most precise ODE solver in MATLAB. While the NDF/BDF calculation method reaches the same results it can be stated that the NDF/BDF method is fast and precise enough for reliable online process simulation with the applied EAF process model. A comparison of the simulation results between the different Euler and BDF/NDF implementations show similar curve shapes with variances due to the implementation methods and requirements.

5. Conclusion

In this paper the influence of three different ODE solvers on model estimated process values is investigated by means of calculation accuracy and computational speed. Here, especially the average measured steel bath temperature according to former model validation[6,7] and the dependency on the chosen ODE solving method respectively the chosen time step size for the calculation are used to analyse the simulation accuracy. Using mathematical models to enhance the EAF process has a great potential and has been given considerable attention in the past decade. However, in order to implement the models in parallel to the actual EAF process and to successfully estimate the process values, such as compositions and temperatures of the steel, slag and gas, two main aspects should be taken into account. First, the model needs to be designed and developed to an appropriate level of complexity, including all major mechanisms occurring during the steel recycling process in the EAF. And second, the method used to evaluate the model should satisfy the requirements of desired accuracy and computational speed. The results of the study have shown that different ODE solving methods can be used in order to achieve the required accuracy of the calculations; however, the computation times, which are needed for proper estimation of the values, vary significantly. As has been shown, the simplest method used, i.e. fixed step Euler, shows strong dependence between the calculation accuracy and step size; thus, making it useful for accurate estimation only when small enough step sizes are used or otherwise, the estimated values diverge from the actual and the results become unusable. The consequence of using small step sizes is a long simulation time, exceeding the real time; thus, making the solver inapplicable in online real-time applications. The other two methods investigated, i.e. variable step Runge-Kutta and NDF/BDF, performed better than the fixed step method; however, large deviations in computational times occur as well. Although the Runge-Kutta method evaluated the model almost twice as fast as the Euler method with the smallest step size, its results still cannot be applied in real-time, since the time needed to obtain the results is approximately two and a half times slower than real time. From the estimation accuracy point of view, the NDF/BDF method performed as well as the Runge-Kutta; but, the time needed to evaluate the model was more than one hundred times shorter, i.e. 60 s for approximately 2700 s of simulated process time. For the specific case of the here applied EAF model simulation, the NDF/BDF method proved to be a fast, reliable and precise ODE solving method and therefore the optimal choice with the best possible accuracy to computational speed ratio. Often when the models are used for online process control, combinations of simulation and optimisation techniques are used in order to obtain the best possible action or a result. Knowing that optimisation is a highly time consuming task, using a solving method with short evaluation times is crucial in order to achieve real-time processing running in parallel to the EAF process. To conclude, the selection of the ODE solver has proved to be one of the more important elements when using mathematical models for calculation of the unmeasured

EAF process values. In spite of proper modelling approach and a complex mathematical model, improper selection of the solver can lead to inaccurate calculations; thus, making the overall system unusable in real applications.

Received: April 14, 2015

Keywords: electric arc furnace; EAF; numerical solution method; process modelling; process simulation

References

[1] J. G. Bekker, I. K. Craig, P. C. Pistorius, *ISIJ Int.* **1999**, *1*, 23.
[2] J. M. M. Fernandez, V. A. Cabal, V. R. Montequin, J. V. Balsera, *Eng. Appl. of Artif. Intell.* **2008**, *7*, 1001.
[3] R. D. M. MacRosty, C. L. E. Swartz, *Ind. and Eng. Chem. Res.* **2005**, *21*, 8067.
[4] R. D. Morales, H. Rodriguez-Hernandez, A. N. Conejo, *ISIJ Int.* **2001**, *5*, 426.
[5] V. Logar, D. Dovzan, I. Skrjanc, *ISIJ Int.* **2011**, *3*, 382.
[6] V. Logar, D. Dovzan, I. Skrjanc, *ISIJ Int.* **2012**, *3*, 402.
[7] V. Logar, D. Dovzan, I. Škrjanc, *ISIJ Int.* **2012**, *3*, 413.
[8] P. Nyssen, C. Ojeda, J. C. Baumert, M. Picco, J. C. Thibaut, S. Sun, S. Waterfall, M. Ranger, M. Lowry, *STEELSIM, International Conference Simulation and Modelling of Metallurgical Processes in Steelmaking, 4, METEC InSteelCon* **2011**.
[9] E. T. Turkdogan, *Fundamentals of steelmaking*, Manay, Leeds, GB **2010**.
[10] V. Logar, I. Skrjanc, *ISIJ Int.* **2012**, *10*, 1924.
[11] R. D. M. MacRosty, C. L. E. Swartz, *AIChE J.* **2007**, *3*, 640.
[12] J. R. Dormand, P. J. Prince, *J. Comput. and Appl. Math.* **1980**, *1*, 19.
[13] L. F. Shampine, M. W. Reichelt, *SIAM J. Sci. Comput.* **1997**, *1*, 1.
[14] W. Dahmen, A. Reusken, *Numerik für Ingenieure und Naturwissenschaftler*, Springer Berlin Heidelberg **2008**.
[15] E. Hairer, S. P. Norsett, G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, Springer **1991**.
[16] Y. E. M. Ghobara, *Master of Applied Science*, McMaster University (Hamilton, Ontario, Canada), Department of Chemical Engineering, **2013**.
[17] Y. X. Wang, J. M. Wen, *J. Phys. Conf. Ser.* **2006**, *1*, 143.