

IMPACTS OF INFRASTRUCTURE, TIMETABLE AND PERTURBATIONS IN OPERATION OF DOUBLE-TRACK RAILWAY LINES WITH MIXED TRAFFIC

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ABSTRACT

Delays play a central role in railway operation. They are of great importance both for customers and operators. They are direct measures of quality and reliability and hereby also an important factor for the competitiveness of the entire railway. Indirectly, the delays also affect quantitative factors such as capacity, i.e. the number of trains that can be (practically) operated. For these reasons, analysis of delays and delay propagation is an essential part of railway operations research.

The up-coming deregulation of railway traffic means that completely mixed traffic can be foreseen on the Swedish railway network. This article shows how the delays on a double-track railway line, operated with mixed traffic, are affected by infrastructure, timetable and primary delays. Experimental design, simulation and response surface metamodelling are applied in a multi-factor simulation experiment with nine factors.

The combination of simulation and experimental design makes it possible to draw general conclusions from a limited number of simulated variants and this type of multi-factor analysis is essential to an understanding of the railway as an operational system. The derived metamodels may also be used in different types of planning processes.

The metamodels show that speed and frequency factors have a great impact on delays. Freight train speed and the frequency of service of high-speed trains in particular turned out to be important. Perturbation factors, i.e. entry delays, were found to affect the delays less. Neither does the distance between adjacent overtaking stations in itself affect the delays. However, the inter-station distance still affects delays through interactions with other factors.

Keywords

Double-track, timetable, railway operation, railway capacity, experimental design, simulation, delays, reliability

INTRODUCTION

The railway is a complex operational system with many inter-dependencies. A better understanding of its operational properties is necessary in order to increase utilisation of the existing system and to gain the knowledge needed to construct future railway lines.

The demand for freight and passenger transport is steadily increasing, but investments in infrastructure do not match this increase. It is therefore necessary to find ways to increase utilisation and thereby also the profitability of existing railway lines.

It is also important to increase the railway's competitiveness and make it a more reliable mode of transportation that offers attractive alternatives. Core factors to achieve this are speed, frequency and reliability. The task is thus to offer more trains, running at a higher (average) speed and with greater punctuality. The only way to achieve this is to start with a deep and thorough knowledge of how these factors interact with each other and with other more technical factors.

In many countries different types of traffic have to be mixed on the same track since there are not enough tracks (lines) to separate them. There are also cases where the demand is insufficient for several parallel systems.

One example of this is the two Swedish main lines where freight services are mixed with several patterns of regularly operated passenger services, see figure 1. The mix in itself implies very specific properties for the traffic. Line capacity decreases with speed difference. Higher speed differences also imply more overtaking situations where faster trains overtake slower ones and this results in a lower average speed for slower trains and decreased robustness for the faster trains that become dependent on other trains.

The necessary changes of railway operation, regarding speed, frequency of service etc, mean important changes to the operational conditions for lines operated with mixed traffic. A question of special interest is how the effect of a change in some factors can be compensated by simultaneous changes in other factors so that the required system performance is maintained (or enhanced).

The so called "Additional delay" is a measure that summarizes the operational performance of a railway system in a good way. In this article additional delay is defined as "*the increase in delay, positive or negative, that a service suffers during its travel over a line section.*" Every kind of deviation from the scheduled timetable is regarded as a delay. A negative additional delay corresponds to a case where a delayed service manages to catch up some of its delay so that it has less delay when it leaves the line section. The primary objective of this article is to show how the additional delay is affected by infrastructure, timetable and primary delays, during mixed operation.

A secondary objective is to develop a method of analysis based on experimental design, simulation and response surface metamodelling that captures the complexity of railway operation. After such a development the method can also be applied to find relationships for other operational properties such as running time etc.

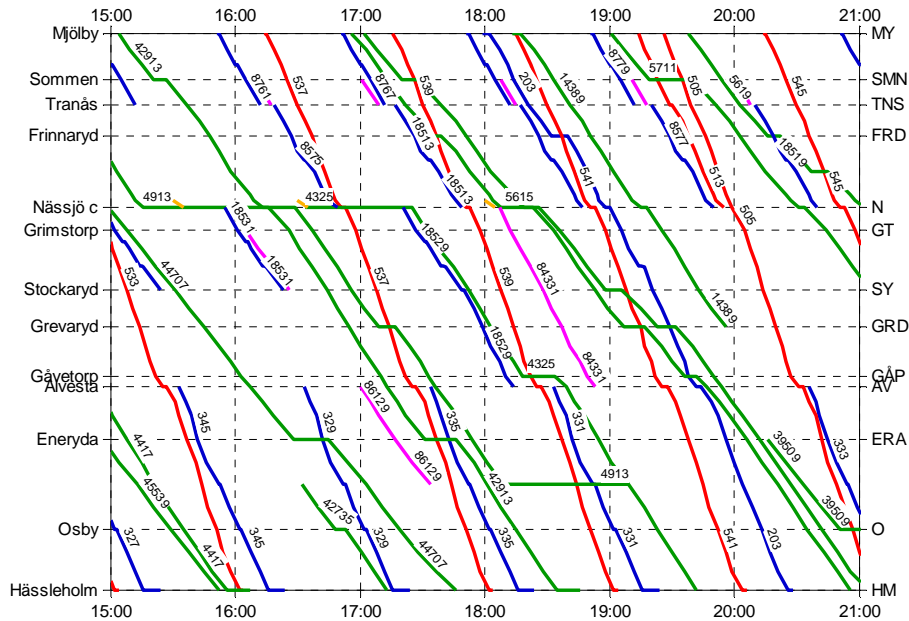


Figure 1: Timetable example from the Swedish Southern Main Line. Upbound services excluded.

The study is delimited to double-track lines operated with a mix of fast passenger services and slower freight services. This implies assumptions about independence between upbound and downbound traffic and that only two speed levels appear. In real operation 3-4 different speed levels on the same track are usual, but in order to obtain transparent results from this first study only two levels are applied.

The study is also delimited to extended lines where the traffic structure remains constant along the entire line and passenger stops are not very frequent. Station areas as well as suburban regions, with additional speed levels (commuter services) and frequent passenger stops, are thus not considered.

Studied factors

A simple, aggregate model, for the additional delay is shown in figure 2.

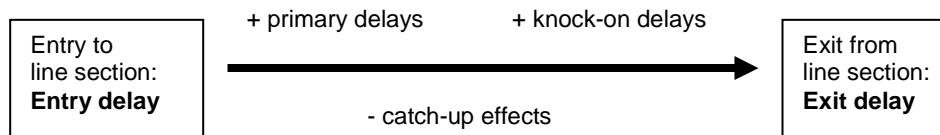


Figure 2: Aggregate delay model for additional delay.

In real operation delays and catch-up effects appear distributed along the line section. It is therefore natural to divide the line section into subsections. The additional delay may then be written as a sum:

$$\text{Additional delay} = \text{Exit delay} - \text{Entry delay} = \sum_{i=1}^k (dp_i + dk_i - c_i)$$

Equation 1: Additional delay.

The *primary delays* depend mainly on the occurrence of vehicle failures, infrastructure malfunctions and dwell time extensions.

The *knock-on delays* are heavily dependent on the combination of primary delays and timetable, but infrastructure and dispatching factors are also important.

The *catch-up effect* implies that a service manages to reduce its delay through the use of margins that are included in the timetable. This effect is complex and also depends on other factors such as traffic mix, vehicle performance and driver behaviour.

All three terms in the sum are stochastic. The randomness of the additional delay can be represented by a distribution that can be described through percentile values or through mean and variance measures.

The competitiveness factors, i.e. frequency of service, speed and occurrence of primary delays all affect the additional delay either directly or indirectly. In this study these factors are divided into three groups:

- Infrastructure factors
- Timetable factors
- Perturbation factors

Mixed traffic on double-track lines is generally operated with overtakings, where faster trains overtake slower ones at main stations and/or at minor overtaking stations. This increases capacity at the cost of scheduled delays for the slower trains.

The locations and density of these overtaking stations affect capacity and operational quality factors. The distance between adjacent overtaking stations is therefore an important factor to evaluate, since a greater number of overtaking stations is likely to decrease the additional delay through better dispatching possibilities.

The timetable example in figure 1 showed that the traffic mix varies over time. The passenger services are often scheduled in periodic timetables. At peak periods the frequency of these services is often increased to meet the higher demand. Freight traffic is less regular, but on several lines it tends to increase in intensity in the late afternoon. From this it is clear that several different combinations of traffic load are of interest, i.e. that several timetable variants should be evaluated.

Perturbations, in the form of entry delays at the origin station and primary delays that appear along the line, also affect the additional delay. A reduction of these perturbations would help to increase the railway's attractiveness both directly through higher reliability and indirectly through the capacity increase that follows from lower margins in the timetable. All together this gives nine factors:

Infrastructure factor:

- Distance between overtaking stations

Timetable factors:

- Speed of high-speed services
- Speed of freight services
- Frequency of high-speed services
- Frequency of freight services

Perturbation factors:

- Entry delays for high-speed services
- Entry delays for freight services
- Primary delays for high-speed services
- Primary delays for freight services

Since this type of complex system cannot be described through simple analytical methods, simulation is an appropriate method to find relationships between these factors and the additional delay.

In a simulation model it is possible to construct and evaluate different infrastructure layouts and timetable designs. It is also possible to assign different kinds of stochastic perturbations to the services. Through detailed modelling of the dispatching function knock-on delays are modelled at a high level of detail. The catch-up effect is handled through stochastic running times.

For this study a simulation model was set up in the simulation tool RailSys. The preceding calibration and validation work was extensive and is described in greater detail in Lindfeldt and Sipilä (2009).

Outline of the article

After this introduction the related research is reviewed (section 2). Thereafter, the method of analysis is described in more detail (section 3). The experimental design will be shown with factor levels chosen to represent the evaluation space of interest. An overview of the simulation model used to perform the experiments will be given, followed by a presentation of the resulting response surface metamodels that describe how the mean and standard deviations for additional delays depend on the nine factors. The adequacy of the metamodels will also be examined.

In section 4 the metamodels are used to illustrate the impact of the factors and the results are further discussed and explained. In section 5 conclusions are drawn, both from the method and from the results.

RELATED RESEARCH

This work covers several different areas of research. The base is railway operation and simulation of railway operation. Theory of experimental design and response surface methods also apply.

The approaches for modelling of railway operation can be divided into analytical, combinatorial and simulation techniques, cf. Mattsson (2007). Queuing theory dominates among the analytical approaches. This type of model was first introduced for railway capacity analysis by Schwanhäusser (1974). He makes a general analysis of buffer times based on queuing theory. He includes a number of factors such as initial delays, supplements, mix of priority classes, punctuality, headways and overtaking possibilities (infrastructure). The buffer times are either constant or exponentially distributed.

Schwanhäusser (1981) analyses overtakings in detail, using probability methods. Exponentially distributed buffer times are also assumed here. The evaluation is divided into two important steps: evaluation of expected value of scheduled delay due to one single overtaking and evaluation of the overtaking frequency, i.e. number of overtakings/hour. The study does not explicitly address capacity problems but provides useful results regarding how scheduled delays depend on speed differences, traffic intensity, mixing ratios and distances between adjacent overtaking stations.

Wendler (2008) has recently provided a general introduction to capacity analysis based on queuing theory. He considers both scheduled waiting times and knock-on delays and emphasises the usefulness of queuing theory for long and medium term studies, where the requested train paths are not known in detail. He concludes by stating that queuing models are not completely suited for cases with a heavily dependent arrival process that follows from periodic timetables.

Yuan and Hansen (2007) develop a stochastic model for estimation of delay propagation at stations. Several factors are modelled stochastically and different operational situations are handled through calculations of conditional probabilities. The method can be used to determine the maximal frequency of trains given an accepted level of knock-on delays.

A major challenge for analytical models is to capture the effect of several sources of primary delays, interactions between trains, dispatching, run time variations, etc. Several of these effects are disregarded, or handled in a simplified way, in the analytical models.

Combinatorial methods are well-suited for analysis of railway systems that are operated with a periodic timetable. Most of the literature, however, focuses on synchronisation and optimisation within networks. The main goal is often to minimise resources (rolling stock, staff etc) and waiting times for passengers who need to change trains.

Liebchen and Möhring (2002) and Liebchen (2004) use PESP (Periodic Event Scheduling Problem) to show that optimisation methods can be used to find periodic timetables that need a minimum number of vehicles and give short waiting times for changing passengers. Nachtigall (1996) provides an improved branch and bound approach to find a timetable such that the arising changing time is minimal for selected stations.

Lindfeldt (2009) proposes a pure combinatorial method for evaluation of capacity on double-track railway lines with mixed traffic. This method does not take perturbations, dispatching and run time variations into account.

Simulation approaches are used within a wide range of applications. They are especially useful for analysing complex technical systems. Law (2007) gives a good introduction to simulation analysis. He emphasises that simulation is “numerically exercising of a model for the inputs in question, to see how they affect the output measures of performance”. Law describes several aspects of simulation. One that applies well to this work is that of probability distributions. Here, he gives useful recommendations concerning empirical and analytical distributions for delay assignment.

Simulation has come to be increasingly used in the field of railway operation in recent decades. Siefer (2008) describes the state-of-the-art as regards railway operation simulation, emphasising the main advantages, i.e. to perform changes and evaluate changes in infrastructure, timetable, rolling stock, delays and/or dispatching strategies, along with discussions of important areas of use, such as planning, timetable construction, robustness analysis, operation etc. Siefer (2008) also underlines the advantages of synchronous simulation models where all events happen in the same order as in reality. Synchronicity is an important condition for a dynamic dispatching algorithm where the priority of the trains shifts according to changes in their status

Lindfeldt and Sipilä (2009) show how a simulation model in RailSys is calibrated against real operational data. A multi-factor calibration was performed for a double-track section with mixed traffic and shows how time supplements are to be utilised by the model, how run time extensions shall be applied and how the dispatching algorithm is to be set.

Time supplements and buffer times are essential in timetable construction. Rudolph (2003) makes a survey of disruptions and disturbances that occur in railway operation. She states that the allocation of time supplements and buffer times at stations is essential to achieve a robust operation. Using simulation she evaluates different allocations of supplements and buffer times. Her conclusions are that both supplements and buffer times should be allocated according to the occurrence of primary and knock-on delays. The allocation process therefore has to be based on information from previous operation and/or simulation studies.

Perturbations are important in railway operation analyses. Yuan (2006) performs a detailed statistical analysis of real-world track occupation and release data to find feasible distributions for delays. He shows that log-normal distributions are best for modelling of arrival times, whereas Weibull distributions are the best choice for non-negative departure delays and dwell times at stations. These are important results since they show that the negative exponential distributions commonly used in simulation experiments mean a simplification.

One advantage of simulation is that the operator can control many factors. Using simulation for multifactor analysis, however, calls for careful planning. Barton (2004) and Sanchez (2007) provide ideas on how simulation experiments can be efficiently performed. They state the dependencies between the response surface metamodel and the experimental design needed to support the desired metamodel. Several examples of designs are described and the importance of interaction effects between factors are underlined.

Kleijnen et al (2005) point out that simulations are very well suited for experiments, but that the experimental designs need to be adjusted for multi-factor analysis. They also discuss the importance of orthogonality, which simplifies computations and makes it easier to determine whether to include a factor in the metamodel or not.

The advantages of space-filling designs are also described. Here the design samples not only at the edges of the hypercube that defines the experimental area, but also in the interior. A design with good space-filling properties means that the analysts need not make many assumptions about the nature of the response surface. Space-filling designs also provide flexibility when estimating a large number of linear and nonlinear effects, as well as interactions, and so provide bias protection when fitting metamodels of specific forms. Kleijnen et al (2005) recommend the so-called *Latin Hypercube* experimental design when many factors are involved and minimal assumptions about the response surface can be made beforehand.

Cioppa and Lucas (2007) describe the properties of *Latin Hypercubes* in detail and present an algorithm for constructing nearly orthogonal *Latin Hypercubes*, given a fixed sample size. They also present a method that improves the space-filling properties of a *Latin Hypercube* at the expense of inducing small correlations between the columns in the design matrix.

Myers and Montgomery (2002) treat *Response Surface Methodology* in detail. They recommend a first-order model as the first step in an analysis, but emphasise that a second-order model is very flexible since it can take on a wide variety of functional forms, so that it will often work well as an approximation to the true response surface. Myers and Montgomery also point out the importance of including interaction effects in the metamodel.

METHOD

The aim of this study is to determine how the additional delay depends on infrastructure, timetable and perturbation factors for mixed traffic operation of double-tracks. This means that several combinations of factor levels must be examined, many of which are located far from the region where Swedish railways are operated today. The method must therefore be chosen and designed with care.

Figure 3 shows how knowledge from existing operation was used to calibrate and validate a simulation model and to generate ideas about the operational space that forms the possible modes of operation for the system.

Once the operational space, i.e. factors and levels belonging to them, had been chosen, the experiment was set up using *Experimental Design* theory. The calibrated simulation model was then used to model the complex railway operation, i.e. perturbation assignment to services, the interaction between services (resulting in knock-on delays), vehicle and driver behaviour, catch-up processes etc.

Regression analysis was then applied to find Response Surface Metamodels (RSMs) from simulated response values and input factor values. After adequacy checks these RSMs can be used to draw conclusions about the impact of the different factors on the additional delay. The nine factors were chosen according to the prevailing situation on the Swedish railway, i.e. an ambition to increase speeds and frequencies of services on existing lines, both for passenger and freight. This made it reasonable to limit the number of factors describing the infrastructure and focus on factors related to timetable and perturbations.

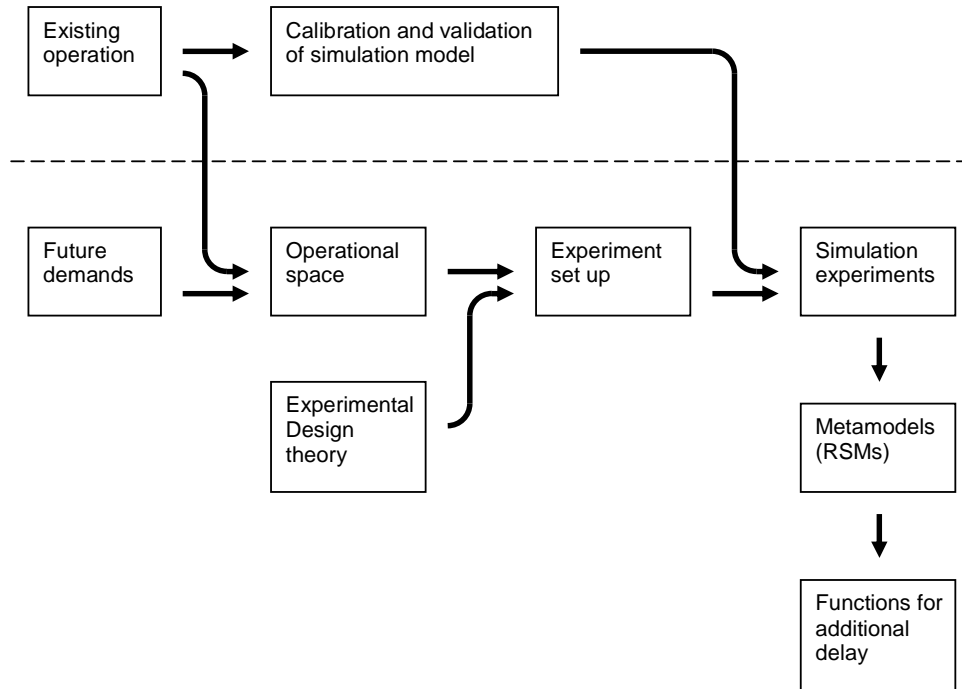


Figure 3: Working scheme for the study.

The infrastructure was therefore represented by only one factor:

x_1 : distance between adjacent overtaking stations 10 – 20 km

The existing inter-station distance in Sweden is about 25 km on average, and so a decrease to 10 km means a major investment in additional overtaking stations.

The development of the Swedish railway operation makes it reasonable to describe the timetable with four independent factors:

x_2 : speed of high-speed services	160 – 225 km/h
x_3 : speed of freight services	90 – 120 km/h
x_4 : frequency of high-speed services	1.0 – 2.0 trains/h
x_5 : frequency of freight services	2.5 – 4.0 trains/h

The speed of high-speed services was assumed to be average speed, including passenger stops every 100 km; the speed of freight services was assumed to be cruising speed without scheduled delays for overtakings.

For simplicity, and since this was a first attempt to derive the desired type of relationships, only one type of passenger service was used. The frequency of this passenger service was assumed to represent the resulting frequency of a real mix of several services.

Two types of perturbation were applied for each service type: entry delays and run time extensions:

x_6 : entry delays for high-speed services	2.5 – 6.0 min
x_7 : entry delays for freight services	14 – 23 min
x_8 : run time extensions for high-speed services	0.5 – 1.0 min/35 km
x_9 : run time extensions for freight services	0.5 – 1.5 min/35 km

The entry delays correspond to everything that causes a delay to services upstream of the modelled line section, whereas run time extensions are primary delays that impact the services along their run through the model. The four factors are actually not single values, but entire distributions from which samples are drawn and assigned to the services during the simulation. The factor values shown above are shape parameters for these negative exponential distributions, i.e. mean values.

During real operation the delays of consecutive trains are not independent. In order to reduce the number of factors, correlations between the values behind the four distributions were sought in delay statistics from real operation. However, such correlations could not be found and so the perturbations had to be represented by four independent factors.

The interval for the perturbation factors were chosen as +/- 0.5 standard deviation from real operational mean values, see Lindfeldt (2008).

Experimental design

The operational system that was to be modelled is a multi-factor system with only quantitative factors, most of them having many possible levels. The shape of the response surface metamodels (RSMs) was not known beforehand.

All these circumstances made the so-called *Latin Hypercubes* (LH) a good design alternative, see Kleijnen et al (2005) and Cioppa and Lucas (2007). These designs have good space-filling properties, but require much less sampling than the corresponding factorial designs. LH support different types of RSMs, including higher order main effects and interaction effects. This is important since both quadratic effects and interactions can reasonably be expected to appear in complex systems such as this.

In LH each of the k factors takes N different levels $\{1, 2, \dots, N\}$. Each column is permuted so that each of the k factors will be sampled exactly once at each of its N levels. The assignment of factor levels was performed by *NOLHdesigns worksheet*, see Sanchez (2005), and so the columns are nearly orthogonal, which increases the efficiency of the design. The entire experiment setup for the 66 design points is shown in the appendix.

All factors except the infrastructure were assigned on 33 different levels. In order to achieve equivalent modelling of the signalling system the infrastructure was only modelled on seven different levels. The levels of the frequency of high-speed services were slightly adjusted compared to the design worksheet, in order to achieve constant scheduled delays for freight trains in overtaking situations. This was necessary since this scheduled delay strongly affects the catch-up effect and thereby the additional delays for the freight trains.

The experiment was performed in two steps. In the first, 33 different design points were chosen over the entire evaluation space. For greater accuracy, a second step was added. In this step, with 33 additional design points, the factors for speed and entry delays were concentrated to the central part of the original evaluation space.

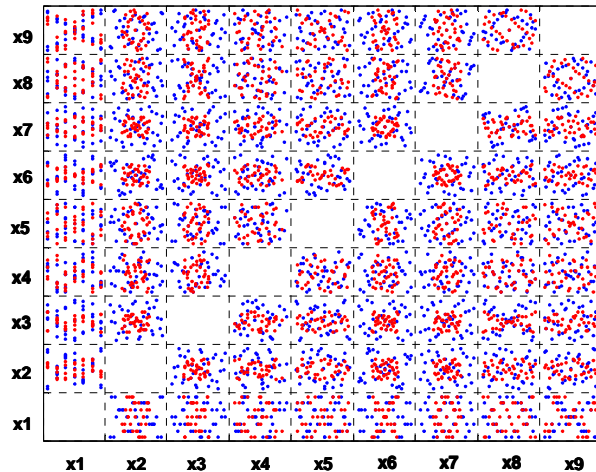


Figure 4: Scatterplot matrix for the Latin hypercube used in the study. Each square shows the space filling in two factors.

The factors are enumerated as shown in the previous section. Figure 4 provides a check of the design's space-filling properties. It is clear that the 66 design points show a satisfactory two-dimensional space-filling behaviour. However, the seven distinct levels of the infrastructure factor, x_1 , decreases the space filling since it results in structured rows/columns. Blue dots represent design points in the first step and red dots design points in the second.

Simulation

The 66 design points (operational cases) were set up in the simulation tool RailSys version 6.3 (Radtke 2005). Values for parameters controlling the catch up effect and the dispatching algorithms were taken from the calibration work presented in Lindfeldt and Sipilä (2009). Hence, in every dispatching situation priority was given to high-speed services for freight services. Overtakings were restricted to overtaking stations and so no "flying overtakings" with parallel operation between stations were modelled.

The infrastructure was modelled as a 275 km line without any gradients and with equally distributed overtaking stations with one side track each. The modelled signalling system corresponds to ETCS level 2 (Wendler 2009), with discrete block sections of standard length. Representative vehicle characteristics were chosen for the two train types used in the analysis, see the appendix for details. All design points were operated with these train types, though with different top speeds according to the speed factors.

For each design point the timetable was given by the infrastructure factor, the two speed factors, the two frequency factors and the vehicle characteristics. The high-speed services were operated periodically and the freight services were spread as evenly as possible in-between according to their prescribed frequency.

Entry delays were assigned to the services at the origin station and run time extensions were applied at subsections every 35 km. The use of run time extensions is further described in Lindfeldt and Sipilä (2009). For each design point the number of replicates (simulated days of operation) was adjusted to give approximately 20,000 evaluated freight services when the warm-up period was deduced. This gave a random relative error of less than 4%.

RESULTS

The results from the simulation experiments are shown in figure 5. The figure gives a first idea about the response variables: mean and standard deviation of additional delay for high-speed and freight services respectively.

It can be seen that the freight services tend to catch up delays, i.e. the catch-up effect is greater than primary and knock-on delays, which result in negative mean additional delays. A high variance between different design points indicates a dependency of the operational factors. It is also noticeable that the standard deviation of additional delay for freight services is high but shows less fluctuation.

High-speed services suffer additional delay in all design points but two. For these services the catch-up effect is less than the primary and knock-on delays that appear during the operation. The high-speed services also show significant fluctuations, indicating a dependency on the operational factors.

Figure 5 also shows that mean and standard deviation tend to follow each other, which is normal in railway operation, see Nelldal et al (2008) and Lindfeldt (2008). A strong interdependency between freight and high-speed services is also evident since all four curves follow each other. Five design points stand out: 2, 16, 20, 35 and 59. In all these points the speed difference between high-speed and freight services is high, as is the traffic load.

In order to evaluate the effect of the nine operational factors the simulated responses were used for regression analysis to derive response surface metamodels.

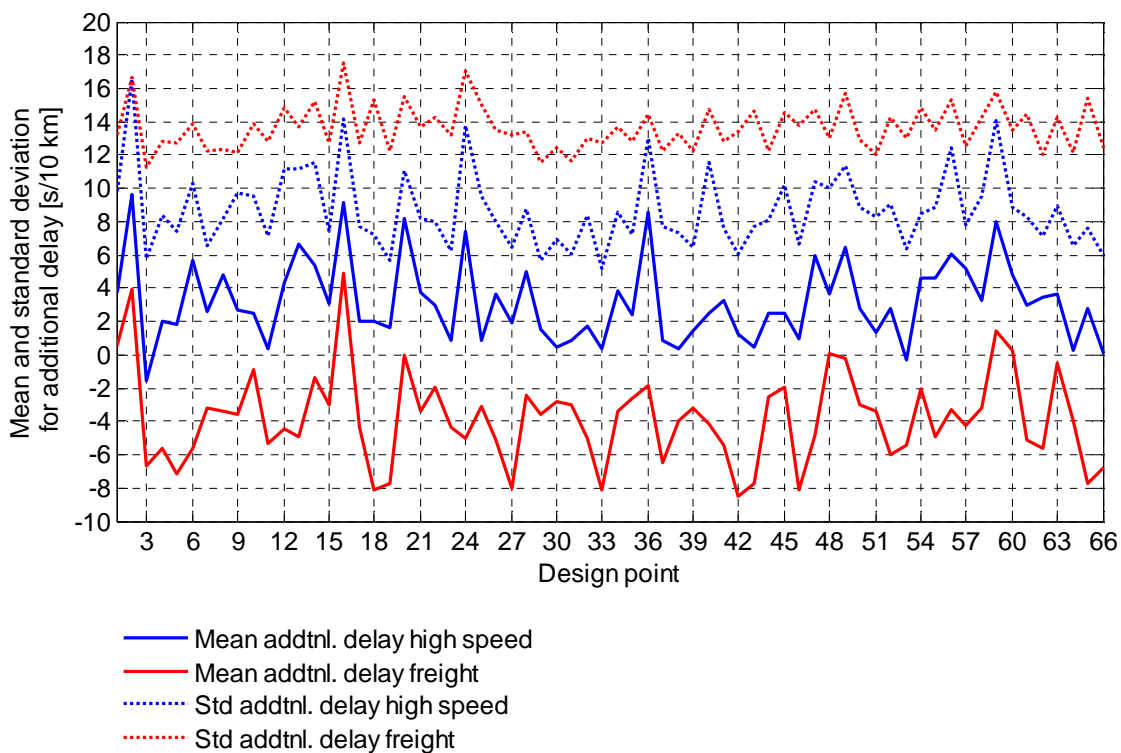


Figure 5: Results from simulation experiments.

Response surface metamodels

Stepwise multi-linear regression was applied to fit a metamodel to each of the four responses:

- Mean additional delay for high-speed services
- Mean additional delay for freight services
- Standard deviation of additional delay for high-speed services
- Standard deviation of additional delay for freight services

The idea of the metamodels (polynomials) is to perform estimations in non-simulated points and to determine the influence of different factors. In the stepwise procedure all first and second order main effects were tested, as well as all two-way interaction effects. Only significant effects were included in the final metamodels. A complete expression for the metamodels is shown in equation 2.

$$y_k = f_k(x_1, x_2, \dots, x_9) + \varepsilon_k = \beta_{k,0} + \sum_{i=1}^9 \beta_{k,i} x_i + \sum_{i=1}^9 \beta_{k,i,i} x_i^2 + \sum_{i=1}^8 \sum_{j=i+1}^9 \beta_{k,i,j} x_i x_j + \varepsilon_k$$

Equation 2: Response Surface Metamodel.

In this expression y_k denotes the response, i.e. the mean or standard deviation of additional delay for a service type. All β :s are coefficients found in the regression analysis. $\beta_{k,0}$ is the constant term, $\beta_{k,i}$ are the coefficients for linear main effects, $\beta_{k,i,i}$ are coefficients for quadratic effects and $\beta_{k,i,j}$ are coefficients for two way interactions. The values of all β :s are tabled in the appendix and shown in figures 7 and 11 below. The x_i :s are coded variables, i.e. transforms of the natural variables, dimensionless and with mean zero. This transformation is described in the appendix.

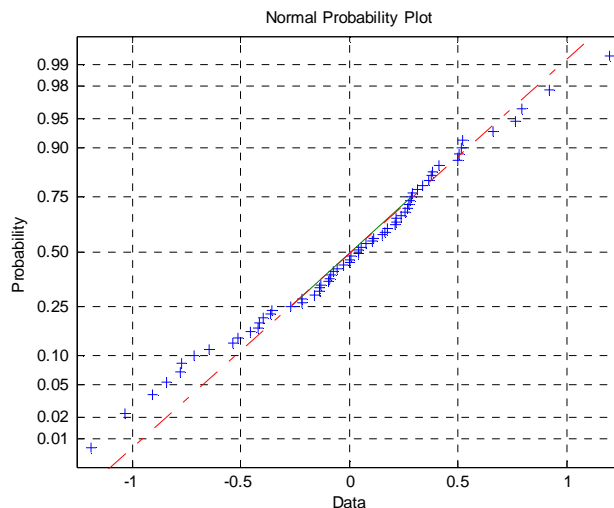


Figure 6: Normal probability plot for high-speed services' mean additional delay.

Residual analysis was performed to check the adequacy of the models. Normal probability plots did not reveal any problems concerning the normality assumption in the regressions, see figure 6 for an example.

Neither did any of the standardized residuals indicate that any observation could be characterized as an outlier. High-leverage points, i.e. observations that have disproportionate leverage on the parameter estimates, were also sought. A few high-leverage points were found, in particular for the mean additional delay model for freight services. The R^2 -statistics for the models were calculated according to definitions in appendix and the values are shown in table 1.

Table 1: R^2 -statistics for the models.

Model	Description	R^2	R^2_{adjusted}	$R^2_{\text{prediction}}$
1	Mean additional delay high-speed	0.9628	0.9516	0.9307
2	Mean additional delay freight	0.9506	0.9394	0.9213
3	Std for additional delay high-speed	0.9519	0.9421	0.9218
4	Std for additional delay freight	0.8664	0.8477	0.8262

The ordinary R^2 measures show that the estimated models fit the responses from the simulated design points well. The metamodel for freight services' standard deviation shows a less good fit than the others.

Adding variables to a model will always increase R^2 , regardless of whether the additional variable is statistically significant or not. To check this, the R^2_{adjusted} measures were also calculated. Since they do not differ dramatically from the ordinary R^2 , the conclusion is that there is a good chance that the models are free from non-significant terms.

The $R^2_{\text{prediction}}$ measure gives an indication of the predictive capability of the regression model. It can be seen that the models are slightly worse at predicting new observations than at explaining variability in the original data.

The standard errors of predicted responses were also estimated. This measure is unique for every point that is to be predicted. These measures are therefore presented in the following sections, together with the predicted additional delays for different factor level combinations.

Additional delays for high-speed services

Figure 7 shows the values of the coefficients in the two metamodels for high-speed services. The numerical values of the coefficients, including the constant terms are listed in the appendix. All coefficients refer to coded variables (x_1 - x_9).

A first conclusion is that if all factors are set to their intermediate level (0) the additional delay becomes 2.5 s/10 km with a standard deviation of 8.7 s/10 km. This operational condition corresponds fairly well to the condition under which Swedish railway lines are operated today (2009).

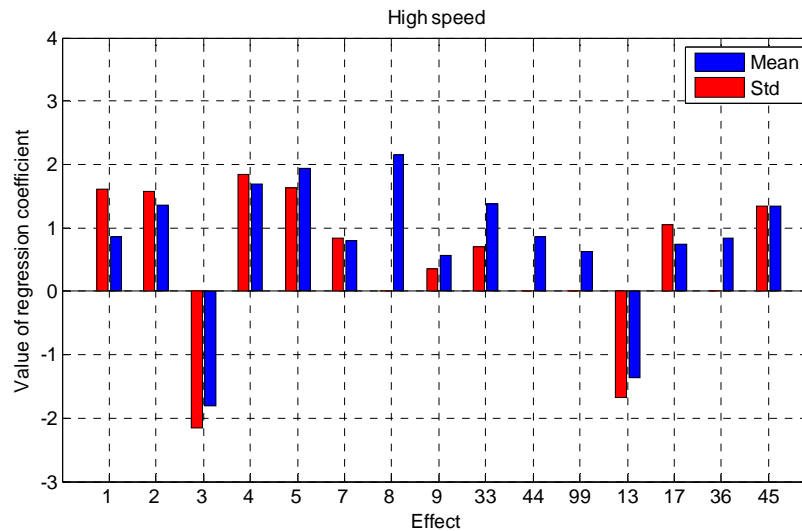


Figure 7: Coefficients for metamodels for high-speed services.

Figure 7 also shows the impact of the analysed factors. Effects 1-9 correspond to linear main effects of factor 1-9, 33-99 are the corresponding quadratic effects and 13-45 are the interaction effects. Factor 6, entry delay for high-speed services, has no significant impact on the additional delay. This means that the dispatching principle, saying that high-speed services shall always be prioritised over freight services, works and that the available capacity is sufficient for this dispatching principle to be fully applicable. It is, however, remarkable that the entry delay shows up in an interaction with factor 3, speed of freight services.

As expected, factor 8, run time extensions for high-speed services, turns out to be highly important. This factor is connected to the primary delays in equation 1.

All factors related to the timetable, factors 2-5, controlling speeds and frequencies, play important roles. The speed of freight services and frequency of high-speed services, factors 3 and 4, also appear as quadratic main effects.

The infrastructure, factor 1, does not seem to be very important for the high-speed services, as far as mean additional delay is concerned. However, the impact of the infrastructure is heavily depending on the speed of freight services and their entry delays (interactions 13 and 17).

The model for the standard deviation is generally less complicated with fewer terms. In this case, however, the infrastructure is much more important. This is seen in a strong first order main effect and interaction effects (13 and 17).

It is impossible to show the ten-dimensional response surface on paper. Instead, any analyst can use the models to estimate the effect in subspaces of special interest. In this article, only three examples that apply for the Swedish railway are shown. No formal analysis of the metamodels, including ridge analysis and search for stationary points, is therefore made.

The chosen examples concern the sensitivity to speed levels, frequencies and infrastructure. The idea is to show how different speed and frequency ratios affect the additional delays. The effect of infrastructure changes is also explicitly addressed. In figures 8 and 9 the metamodels are used to estimate the effect of different speed and frequency combinations. In both cases all other factors are set to an intermediate level.

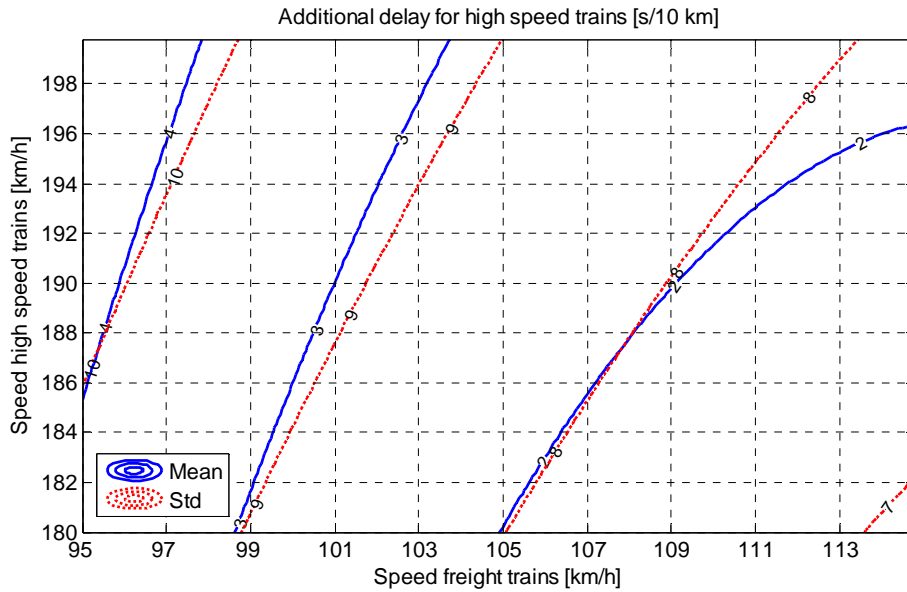


Figure 8: Additional delays for high-speed services at different speeds.

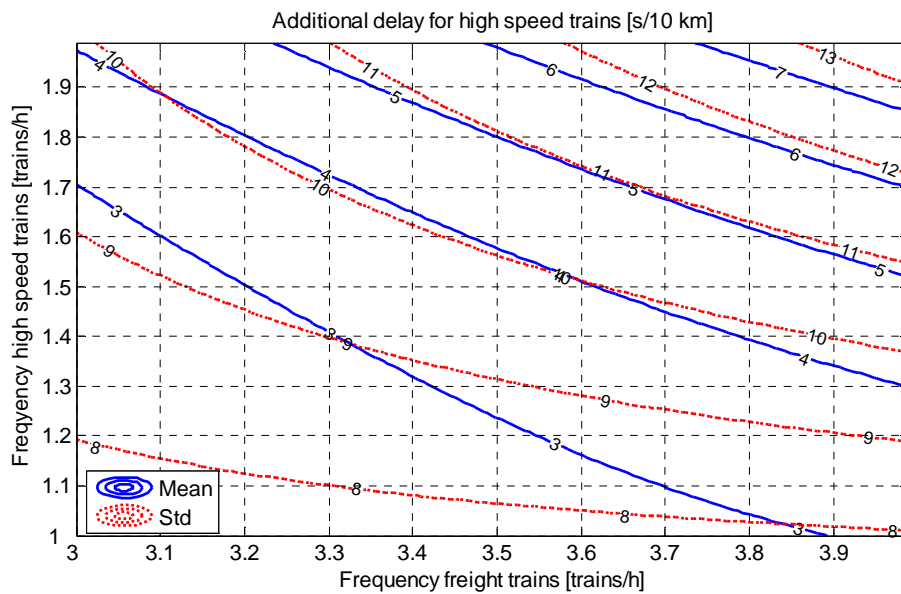


Figure 9: Additional delays for high-speed services at different frequency of service.

Figure 8 shows that higher speed for high-speed services results in longer delays, whereas higher speed for freight services results in shorter delays. The slopes of the lines show that the impact of freight speed is greater. Due to the quadratic effect for freight speed (33) both lines for mean and standard deviation are curved.

Figure 9 shows the effect of different frequency of service. In this case both increased high-speed frequency and increased freight frequency result in greater delays. The contour lines

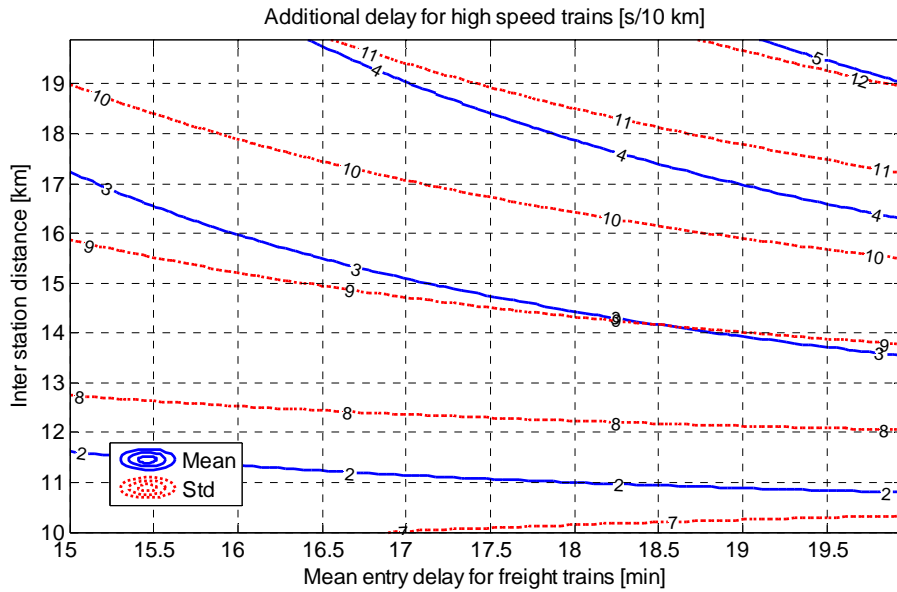


Figure 10: Additional delays for high-speed services at different inter-station distances and entry delays for freight trains.

are closer together for higher frequencies. This indicates the saturation phenomenon that occurs when traffic increases.

The standard deviation shows the same pattern as the mean, and so the delay variance increases with frequency of service.

The slopes of the lines show that the impact of high-speed frequency is greater than the impact of freight frequency. Both mean and standard deviation lines are curved. This curvature is due to the quadratic effect (44) and the interaction effect (45), see figure 7.

The additional delay also depends on the infrastructure. Shorter inter-station distances mean better possibilities to take dispatching actions that limit the knock-on delays. Figure 10 shows how the inter-station distance and the entry delays for freight trains affect the additional delay for high-speed services.

It is remarkable that the additional delay is not more sensitive to entry delays. For short inter-station distances the additional delay is almost independent of the freight trains' entry delays. In this case the number of available overtaking stations is so high that even heavily delayed situations can be handled by dispatching.

Both mean and standard deviation lines are curved. This curvature is caused by the interaction effect (17). The standard deviation lines are denser and hence the inter-station distance is more important for variance than for the mean additional delay.

Additional delays for freight services

The freight services face a different situation. Although they suffer from higher entry delays, greater run time extensions and lower priority than the high-speed services, they generally tend to catch up delays. This is due to the time supplements that are introduced at each overtaking.

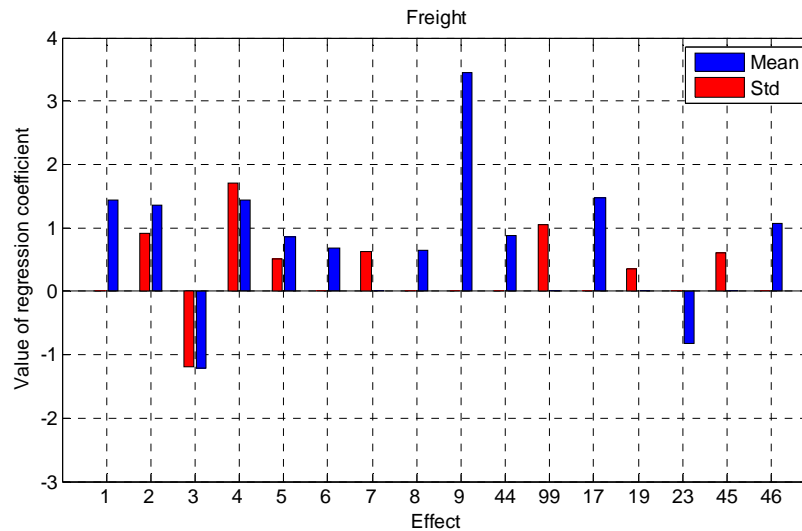


Figure 11: Coefficients for metamodels for freight services.

Figure 11 shows the values of the coefficients in the two metamodels for freight services. Effects 1-9 correspond to the linear main effects of factors 1-9, 44 and 99 are the corresponding quadratic effects and 17-46 are the interaction effects. The numerical values, including the constant terms, are listed in appendix. All coefficients refer to coded variables. If all factors are set to their intermediate level (0) the mean additional delay is -3.9 s/10 km with standard deviation 13.4 s/10 km. These values do not correspond entirely to real Swedish operation. The discrepancy can be explained by the fact that real operation is more heterogeneous with regional services etc.

Figure 11 shows that all factors except the entry delay of freight services (factor 7) affect the mean additional delay. Run time extensions (factor 9) play a very important role. Infrastructure (factor 1), speed (factor 2 and 3) and the frequency of high-speed services (factor 4) are also important.

Significant quadratic main effects occur for high-speed frequency (44) and for run time extensions for freight services (99). The most important interaction effects are shown for infrastructure – entry delay for freight services (17) and frequency of high-speed services – entry delay for high-speed services (46).

The metamodel for the standard deviation is less complicated with fewer terms. The speed of freight services (factor 3) and the frequency of high-speed services (factor 4) strongly affect the variance in additional delays. However, R^2 -statistics reveal a less good model fit for the standard deviation model. This can be explained by differences in the allocated train paths. The number and location of overtakings differ from one path to another. This implies variances that are difficult to explain with only second order response surfaces.

Figure 12 shows that the additional delays for freight services depend on the speed of the two service types. A lower speed difference results in less additional delay (lower right corner), whereas a higher speed difference means more additional delay (upper left corner). The slopes of the lines tell us that the speed of freight services is more important than the speed of high-speed services. If figures 8 and 12 are compared it is seen that speed affects the high-speed services more (denser lines) than the freight services. One explanation for this is that lower speed differences decrease the number of overtakings and so also the time

supplements for the freight services. This reduces the catch-up effect for the freight trains and partly neutralises the effect of lower speed differences. The lines for mean additional delays in figure 12 are curved, whereas the standard deviation lines are straight. This is due to the interaction effect (23) in the mean metamodel (see figure 11).

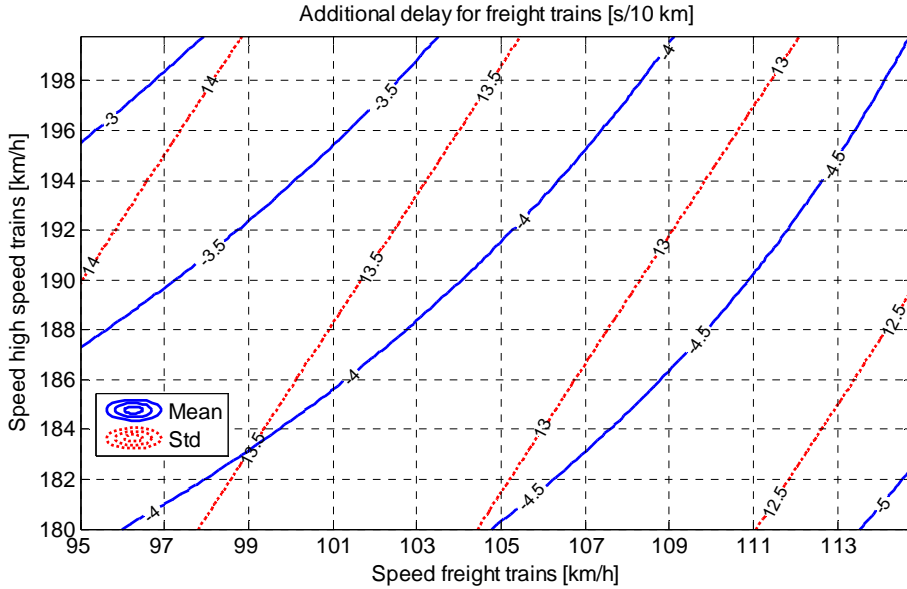


Figure 12: Additional delays for freight services at different speeds.

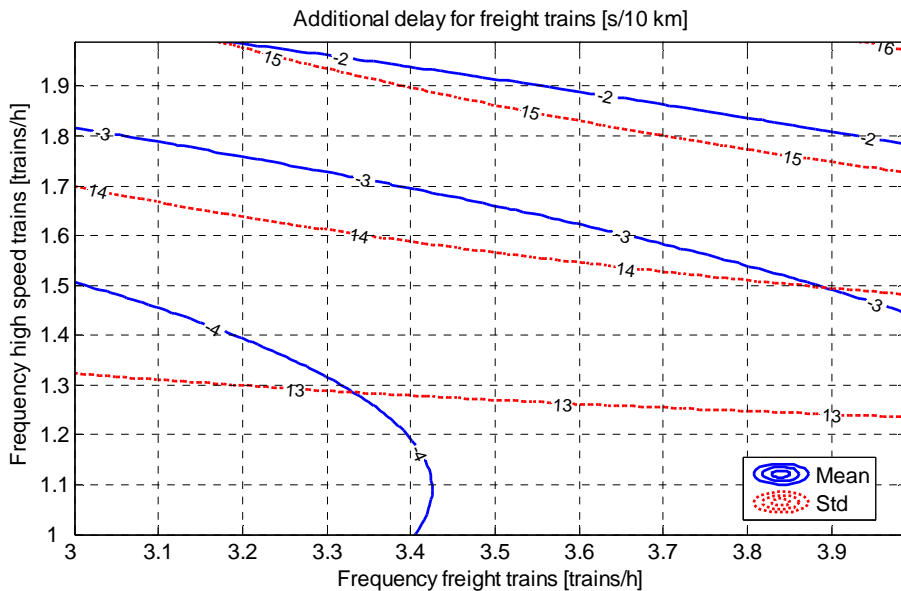


Figure 13: Additional delays for freight services at different frequencies.

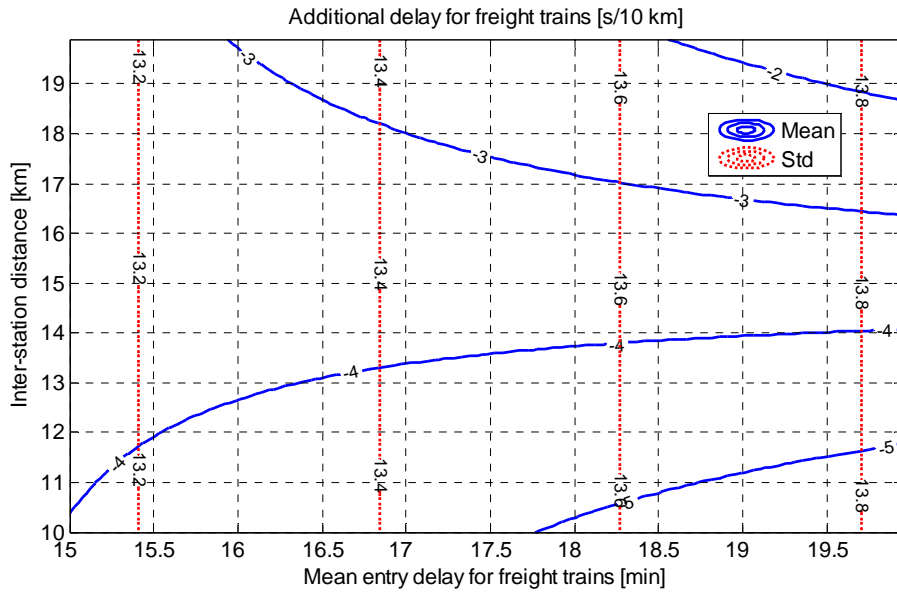


Figure 14: Additional delays for freight trains at different inter-station distance and entry delays for freight trains.

Figure 13 shows that the frequency of freight services does not affect the additional delay very much. However, the frequency of high-speed services is more important. A strong quadratic effect for the frequency of high-speed services (44) is seen in sharply bent lines for mean additional delays. The standard deviation lines are less curved and their curvature is caused by the interaction effect between the two frequency factors (45).

Figure 14 shows two unexpected relationships between additional delay and inter-station distance and entry delays for freight trains. As for the high-speed trains the impact of freight trains' entry delays is very limited. Due to a strong interaction effect (17), for short inter-station distances it is possible to catch up more delays when the entry delay is greater. This follows from the combination of good dispatching possibilities, i.e. many overtaking stations and limited capacity utilisation, and more delay that can be caught up. In the simulation model, freight trains stop catching up delays when they reach their scheduled timetable. The available amount of delay to catch up is therefore greater when the entry delays are greater. The metamodel for standard deviation shows a very weak dependence on entry delays and a complete independence of the inter-station distance (vertical lines).

Standard error of predicted response

A response surface metamodel provides estimations of a response variable. It is important to keep in mind that these estimations possess sampling variability. Standard errors provide a rough idea about the relative quality of predicted response values in various locations in the design region. Hence, they can be used in constructing confidence limits around a predicted response.

The standard error is very much dependent on the experimental design. It is also a function of the model and the location of the point being considered. Figures 15 and 16 show 95% confidence intervals for mean additional delays and standard deviation of delay for high-

speed services. In this case the independent variables are the frequency of the two service types.

Note that the prediction deteriorates as one approaches the design perimeter, whereas the prediction is better in the middle. Since the standard error depends on the location of the considered point, one needs to calculate the error for each point that is of interest. Confidence plots for other examples given in previous sections are omitted here. In general, the metamodels for the freight trains show a somewhat wider interval and less precision.

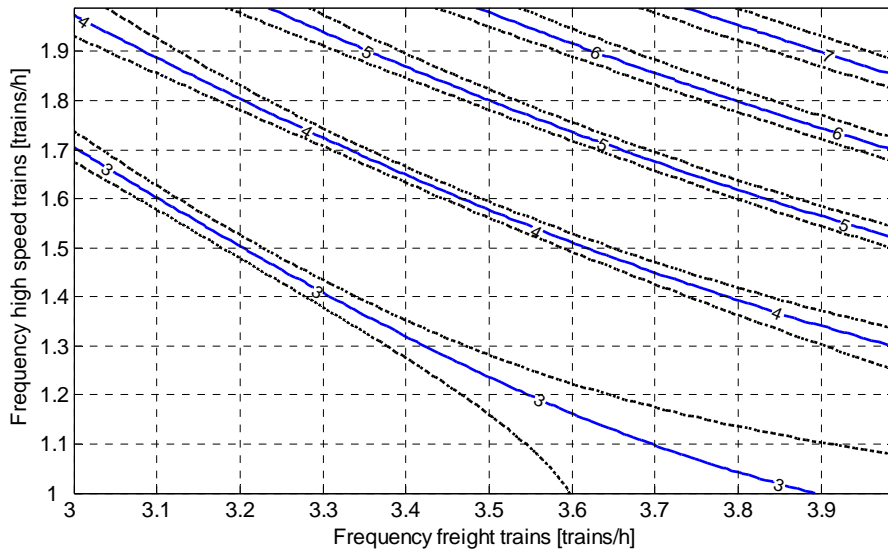


Figure 15: Mean additional delays, including 95% confidence intervals, for high-speed trains at different frequency of service.

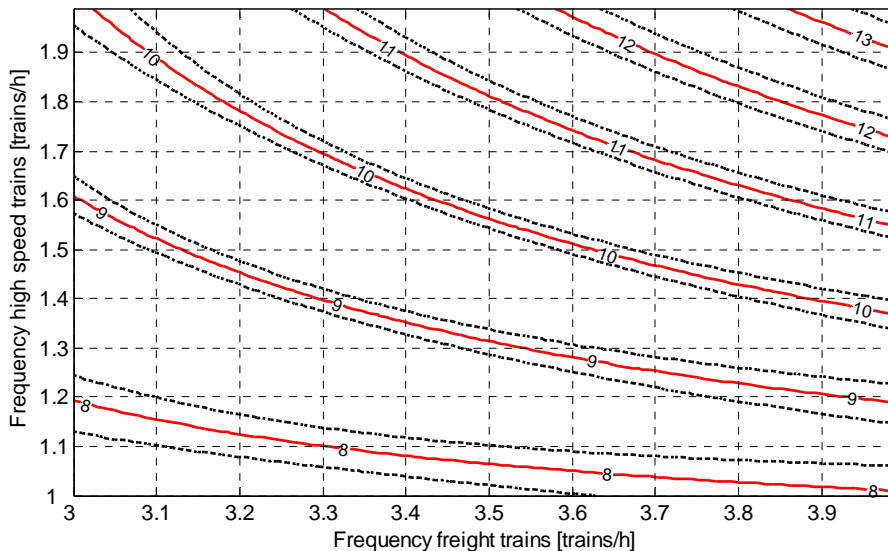


Figure 16: Standard deviation of additional delays, including 95% confidence intervals, for high-speed trains at different frequency of service.

CONCLUSIONS

The railway is a complex system that is difficult to model and analyse. Simulation therefore appears to be an appropriate method for analysis of railway operation. In a simulation tool, like RailSys, it is possible to perform experiments to evaluate the effect of different factors and to model stochastic events such as delays, driver behaviour etc. The advantages of simulation experiments for full-scale experiments are obvious, since changes in railway systems are expensive and not easily performed.

In this study, the real world is therefore replaced by a simulation model, where nine different factors are varied systematically. The results from the simulations are then evaluated by means of response surface methods. This kind of metamodel provides much more information about the underlying system than haphazard investigation of a few variants.

The two main objectives were to determine how infrastructure, timetable and perturbation factors affect the delays that occur along a railway line and to develop a method for such analyses.

Additional delay was chosen as response variable, since it is an efficient measure of railway operation's performance. Other possible response variables might be scheduled run time, mean exit delay and standard deviation of exit delay, or a linear combination of all three.

Methods and experiment setup

In their most simple form, simulation experiments only answer question of the “*what happens if?*” type. Of course it is possible to put a large number of such questions and perform the corresponding simulations to draw conclusions about the system.

The idea of experimental design is to choose the factor levels in each simulation (design point) in such a way that as much information as possible can be extracted from a limited number of simulations. The extraction of information may be performed by means of so-called response surface methodology, where the impact of the studied factors is calculated through regression analysis. In the literature, Barton (2004), Cioppa and Lucas (2007) and Kleijnen et al (2005), the so called *Latin Hypercubes* is a recommended design in cases where the shape of the response surface is unknown and/or more complicated relationships are expected.

Another part of the experiment setup is the choice of factors and the range of each factor. This study focuses on the effect of timetable factors. Factors that define the timetable are thus of special interest. It turned out that real timetables with 3-4 different train types are not easily described with a few factors, not even if the trains are assumed to operate with a regular timetable and at the same frequency. This first study was therefore restricted to only two train types, which gives simpler and more transparent results and opens up for future analysis of more complicated traffic patterns.

Despite this simplification it was rather difficult to describe the timetable unequivocally with just a few independent factors. In fact, inter-station distance, speeds and frequencies cannot be chosen independently if one also requires all overtakings in all design points to have the same amount of buffer time. This requirement is essential to achieve consistency and comparability in the modelling of catch-up effects.

The solution to this problem was to slightly adjust the frequency of the high-speed services to get the required overtaking time. This adjustment, relative to the prescribed values in the experimental design, means that only “ideal” combinations of infrastructure and timetable are analyzed. The interaction effects of inter-station distance, speeds and frequencies, which occur in timetabling, are hereby disregarded.

Primary delays are essential in railway operation and they have a great impact. The perturbations therefore appear as important factors that have to be modelled carefully. The use of negative exponential distributions for the perturbations is a compromise between the number of factors and the accuracy of the model. Literature, i.e. Yuan (2006), shows that both entry delays and run time extensions follow other, more complicated, distributions that require more factors to be modelled.

The infrastructure is represented by one single factor, viz. the inter-station distance. This factor was modelled on a wide range, with a big difference between its minimum and maximum level. Hereby the infrastructure serves as a reference factor to the timetable factors in focus in this study.

The ranges of the factors were chosen with regard to existing values in real operation. The choice of these ranges has a great impact on the metamodelling since they limit the evaluation space and affect accuracy. A balance must be struck between choosing a range wide enough to cover the area of interest and not losing too much accuracy in the (approximating) metamodelling.

The experiment was performed with 66 design points. Care was taken to choose these points according to the experimental design to achieve good space-filling and orthogonality. A lot of experience from the previous calibration of the simulation model, see Lindfeldt and Sipilä (2009), could be utilized in the simulation experiments. This applied in particular as regards modelling of time supplements, buffer times, driver behaviour/catch-up effects, signalling system and primary delays.

High variances in applied delays required a high number of replicates, e.g. number of simulated days of operation, to limit the random error. Unfortunately, variance reducing techniques, such as common random numbers, could not be applied since the perturbation factors implied different sample distributions for delays to be used in each design point. Some of the differences between the design points can therefore be related to the randomization of delays.

The simulation model generally showed consistent results that seemed reasonable. All trains were operated in patterns with a common frequency and this resulted in transparent results and possibilities to detect errors.

The results from the simulations were used to derive response surface metamodelling. These are polynomials that provide good local approximations to the real, unknown, response function. The most simple response surfaces contain only first order terms, which is feasible when the functions are roughly linear over the range of interest. Some of the factors were given wide ranges in the experiment and curved relationships could therefore be expected. To capture this effect both second order terms and interactions were included in the metamodelling.

A stepwise fit procedure was applied to find significant factors. Only these factors were included in the presented final metamodelling. This resulted in 8-15 terms in each model.

Stochastic measures such as delays are most conveniently described by entire distributions. In this study these distributions are represented by mean and standard deviations. This is a simplification since information is lost, but together these measures give a rough idea of the delay level and its variance.

Relatively high R^2 -values indicate that the models fit the simulated results well and that they can predict non-simulated points fairly well. Altogether the methods used in this study, experimental design, simulation and response surface methodology proved to be feasible for analysis of railway operation.

Metamodels and additional delays

The fitted metamodels can be used to estimate the effect of changes in one or several factors. Such estimations are very useful in long term planning, but also when strategies for constructing robust timetables are to be chosen.

The metamodels generally show a fairly high degree of operational robustness for both train types – the additional delays are limited. This shows that the studied traffic mix is not a very big challenge for a double-track railway line, as long as only additional delays are considered.

The freight trains do not suffer any additional delays. Instead they tend to catch-up delays in almost every operational case. This is natural since every overtaking means that time supplements are added in the timetable. These supplements increase the possibilities to catch up delays through shorter stops than planned. It could be argued that actual speed would be a more important measure for the freight traffic. The actual speed is affected both by scheduled delays caused by overtakings, operational delays caused by primary delay sources and conflicts with other trains, and catch-up effects that follow from time supplements in the overtaking situations.

The additional delays for high-speed trains are limited to less than 10 s/10 km. The higher values, 7-10 s/10 km, would certainly imply considerable delay problems, whereas the lower values, 2-4 s/10 km, would be regarded as acceptable. This span in additional delay shows that the evaluated factors actually matter for the high-speed traffic.

All nine factors proved to be significant for the additional delays. Entry delays turned out to be the least important factors. This means that this kind of system and operation is quite independent of the delay level. The focus could therefore be shifted to the other factors in future studies.

As expected both speed and frequency play important roles as regards additional delay. Freight train speed in particular seems to be essential. It appears in linear and quadratic terms and in several interactions. The frequency of high-speed services affects the number of overtakings directly and makes this factor important for the additional delay. This effect is enhanced by a strong interaction between the two frequency factors.

The infrastructure factor, the distance between overtaking stations, affects the additional delay in a complicated way with several interactions. This factor seems to be more important for freight services, probably due to the strict dispatching rule that prioritises high-speed services.

Run time extensions are essential for accurate modelling of railway operation. These two factors also show a significant impact on the additional delays. It is clear that the railway

system would gain from increased reliability in infrastructure and vehicles, more precise and accurate dispatching, less variation in driver behaviour, etc.

This study can be used to screen proposed further studies. It shows that it is possible to disregard all, or at least some of, the perturbation factors in order to focus on the timetable factors. One way to reduce the number of factors even more would be to perform separate analyses of the most interesting frequencies, e.g. one and two high-speed trains/h. Such a reduction would make it possible to analyze a mix with three different speed levels (train types). A delimitation to frequency levels that occur in real operation in combination with a more complicated mix of trains should result in a more realistic analysis.

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APPENDIX

Train characteristics

	High-speed	Freight
Length [m]	155	500
Braking rate [m/s ²]	0.6	0.3
Weight [tons]	360	820
V [km/h]	Acc [m/s ²]	Acc [m/s ²]
	0	0.594
	1	0.594
	10	0.593
	20	0.592
	30	0.591
	40	0.59
	50	0.588
	60	0.586
	70	0.584
	80	0.582
	90	0.552
	100	0.492
	110	0.442
	120	0.4
	130	0.363
	140	0.331
	150	0.302
	160	0.276
	170	0.253
	180	0.231
	190	0.21
	200	0.191
	210	0.173
	220	0.156

Design points

Design point	1	2	3	4	5	6	7	8	9
	Int stn [km]	Speed ht [km/h]	Speed ft [km/h]	Freq ht [trains/h]	Freq ft [trains/h]	Entry ht [min]	Entry ft [min]	Rte ht [min/35km]	Rte ft [min/35km]
1	19.3	166	104	1.1707	3.8157	4.69	20.19	0.73	1.5
2	19.3	224	94	1.2834	3.2307	3.16	20.75	0.66	1.41
3	17.8	188	119	1.1734	2.5641	4.58	20.47	0.52	0.81
4	14.8	216	122	1.4493	3.9087	3.05	21.31	0.53	0.94
5	19.3	162	105	1.2308	3.5604	5.02	17.66	0.78	0.56
6	19.3	220	100	1.2081	3.1767	3.27	15.41	0.94	0.53
7	16.3	190	121	1.2853	2.5262	4.8	17.38	0.95	1.38
8	14.8	204	120	1.3699	3.8886	3.38	15.97	1	1.03
9	16.3	176	97	1.5686	3.6166	3.59	14	0.59	1.09
10	17.8	202	99	1.5632	2.8658	4.36	14.84	0.69	1.34
11	16.3	174	114	2.0501	3.0325	2.72	15.13	0.58	0.88
12	17.8	206	111	1.7991	3.641	5.89	18.22	0.7	0.72
13	16.3	170	96	1.5915	3.3981	2.94	22.72	0.89	0.84
14	17.8	198	102	1.9565	2.7391	4.47	22.44	0.86	0.75
15	16.3	172	117	1.9459	3.0703	2.5	19.91	0.88	1.22
16	17.8	200	109	2.1176	3.7599	5.67	19.06	0.83	1.31
17	14.8	192	106	1.428	3.2887	4.25	18.5	0.75	1
18	10.3	218	108	1.7673	2.7156	3.81	16.81	0.77	0.5
19	10.3	160	118	1.5979	3.3253	5.34	16.25	0.84	0.59
20	11.8	196	93	1.7578	3.9872	3.92	16.53	0.98	1.19
21	14.8	168	90	1.5727	2.6212	5.45	15.69	0.97	1.06
22	10.3	222	107	1.725	2.9756	3.48	19.34	0.72	1.44
23	10.3	164	112	1.6941	3.3448	5.23	21.59	0.56	1.47
24	13.3	194	91	1.8063	4.0427	3.7	19.63	0.55	0.63
25	14.8	180	92	1.776	2.6424	5.13	21.03	0.5	0.97
26	13.3	208	115	1.4932	2.9424	4.91	23	0.91	0.91
27	11.8	182	113	1.277	3.699	4.14	22.16	0.81	0.66
28	13.3	210	98	0.9915	3.5152	5.78	21.88	0.92	1.13
29	11.8	178	101	1.0737	2.9078	2.61	18.78	0.8	1.28
30	13.3	214	116	1.476	3.1257	5.56	14.28	0.61	1.16
31	11.8	186	110	1.1211	3.7671	4.03	14.56	0.64	1.25
32	13.3	212	95	1.1211	3.4531	6	17.09	0.63	0.78
33	11.8	184	103	1.0124	2.817	2.83	17.94	0.67	0.69
34	14.8	181	110	1.6021	3.5507	4.2	20.75	0.84	1.09
35	11.8	187	104	1.2241	3.6285	3.92	20.33	0.72	1.34
36	19.3	180	97	1.5551	3.5853	3.43	17.66	0.98	0.88
37	19.3	188	111	1.1443	3.741	3.48	18.22	0.55	0.72
38	14.8	182	107	1.6909	3.1217	4.36	16.53	0.56	1.19
39	13.3	184	104	1.2097	2.7778	4.91	16.39	0.77	1.25
40	19.3	183	97	1.5339	3.0677	4.96	20.19	0.5	0.78
41	19.3	186	111	1.277	2.8624	5.13	18.64	0.97	0.69
42	11.8	192	108	1.2703	2.5406	3.7	18.92	0.8	0.56
43	13.3	197	100	1.5578	2.6828	4.03	20.05	0.59	0.53
44	17.8	206	102	1.0909	2.7055	3.65	17.94	0.81	1.16
45	16.3	205	108	1.8605	3.245	4.09	17.23	0.58	1.06
46	11.8	193	106	1.1472	3.9712	4.74	17.8	0.64	0.5
47	13.3	203	99	1.5031	3.9081	4.63	17.38	0.89	0.63
48	17.8	204	103	1.0081	3.5065	4.69	19.48	0.67	1.41
49	16.3	207	109	1.8701	3.3488	4.52	19.91	0.88	1.03
50	14.8	191	105	1.5727	3.2765	4.25	18.5	0.75	1
51	14.8	201	99	1.3884	2.9936	4.3	16.25	0.66	0.91
52	17.8	195	105	1.74	2.9145	4.58	16.67	0.78	0.66
53	10.3	202	112	1.4343	2.9555	5.07	19.34	0.52	1.13
54	10.3	194	98	1.8672	2.8225	5.02	18.78	0.95	1.28
55	14.8	200	102	1.3029	3.4311	4.14	20.47	0.94	0.81
56	16.3	198	105	1.8386	3.8055	3.59	20.61	0.73	0.75
57	10.3	199	112	1.3626	3.4724	3.54	16.81	1	1.22
58	10.3	196	98	1.6736	3.6906	3.38	18.36	0.53	1.31
59	17.8	190	101	1.6815	4.0096	4.8	18.08	0.7	1.44
60	16.3	185	109	1.4303	3.9007	4.47	16.95	0.91	1.47
61	11.8	176	107	1.875	3.8372	4.85	19.06	0.69	0.84
62	13.3	177	101	1.0381	3.3399	4.41	19.77	0.92	0.94
63	17.8	189	103	1.7366	2.5615	3.76	19.2	0.86	1.5
64	16.3	179	110	1.5025	2.6187	3.87	19.63	0.61	1.38
65	11.8	178	106	2.0179	3.0484	3.81	17.52	0.83	0.59
66	13.3	175	100	1.1057	3.1843	3.98	17.09	0.63	0.97

Meta models

Factors

1. Distance between adjacent overtaking stations
2. Speed for high-speed services
3. Speed for freight services
4. Frequency for high-speed services,
5. Frequency for freight services
6. Entry delays for high-speed services
7. Entry delays for freight services
8. Run time extensions for high-speed services
9. Run time extensions for freight services

Train type Model type	High speed		Freight		
	Mean	Std	Mean	Std	
Constant term	0	2.5451	8.6562	-3.9219	13.4023
Linear main effects	1	0.8609	1.6142	1.4466	<i>Not sign.</i>
	2	1.3514	1.578	1.3633	0.9246
	3	-1.8058	-2.1677	-1.2106	-1.1953
	4	1.68	1.8445	1.441	1.7086
	5	1.9322	1.6331	0.8636	0.5126
	6	<i>Not sign.</i>	<i>Not sign.</i>	0.6864	<i>Not sign.</i>
	7	0.7947	0.8353	<i>Not sign.</i>	0.6231
	8	2.1567	<i>Not sign.</i>	0.6438	<i>Not sign.</i>
	9	0.5708	0.3565	3.4461	<i>Not sign.</i>
Quadratic effects	33	1.3705	0.7034		
	44	0.8515		0.8761	
	99	0.6257			1.0473
Interactions	13	-1.3699	-1.6689		
	17	0.7467	1.0449	1.4737	
	19				0.3566
	23			-0.8193	
	36	0.8411			
	45	1.34	1.3455		0.5981
	46			1.0618	

If ξ_{ki} denotes variable k at design point i expressed in actual unit values, the corresponding coded variable x_{ki} is given by:

$$x_{ki} = \frac{\xi_{ki} - [\max(\xi_{k\cdot}) + \min(\xi_{k\cdot})] / 2}{[\max(\xi_{k\cdot}) - \min(\xi_{k\cdot})] / 2}$$

R^2 -statistics

Definitions for the three R^2 -measures:

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

$$R^2_{adjusted} = 1 - \frac{SS_E / (n - p)}{SS_T / (n - 1)}$$

$$R^2_{prediction} = 1 - \frac{PRESS}{SS_T}$$

$$PRESS = \sum_{i=1}^n \left(\frac{e_i}{1 - h_{ii}} \right)^2$$

h_{ii} : *hat matrix*