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Automated IC engine model development with uncertainty propagation

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Abstract

This paper describes the development of a novel *data model* for storing and sharing data obtained from engine experiments, it then outlines a methodology for automatic model development and applies it to a state-of-the-art engine combustion model (including chemical kinetics) to reduce corresponding model parameter uncertainties with respect engine experiments. These challenges are met by adopting the latest developments in the *semantic web* to create a shared *data model* resource for the IC engine development community. *Application models* can then access this database to automatically set-up simulations and validation exercises. A methodology for incorporating experimental and model uncertainties into model optimization and final results for multi-parameter and complex modeling applications is presented.

Data from seven operating points have been extracted from the proposed *data model* and have been incorporated into a state-of-the-art in-cylinder IC engine model through the optimization of forty-two model parameters whilst accounting for the model parameter and experimental uncertainties.

Contents

1 Introduction

Exploiting the useful information or *knowledge* held within the vast quantities of experimental data produced during the on-going engine development process is a major challenge for the academic and industrial community. Those that can master these data and can apply the *knowledge* effectively can develop more efficient and low cost engines over shorter timescales. The methodology outlined in this research paper seeks to deliver increased predictive capability and model robustness through automated model development.

"Process Informatics seeks to solve these problems through the integration of hardware, middleware, software, databases, and human resources, all integrated through a network" [1]. An example of a practical working system is the *Process Informatics Model* (*PrIMe*) [2] which is used for the determination of chemical kinetic rates for combustion based on an open-source database written using *eXensible Mark-up Language* (*XML*). The objective was to reduce the uncertainty on model parameters through systematic comparison with fundamental experimental data and a set of computer-based tools to process data consistently from all available data sources. Researchers aimed to systematically identify regions in which the models are unsuccessful, then suggest to the community the most useful future experiments thus resulting in more rapid development timescales [3, 4].

These same aspects are relevant to the problems facing the I.C. engine community, and this model has been adopted to carry out systematic model developments for simple empirical expressions [5]. This research paper describes the continuing implementation of a Process Informatics based model for advancing IC engine development. Details of a web based engine data storage tool and model integration are described, this work builds on previous research activities [5] by firstly extending the *data model* and the complexity of the *application model*, this time a state-of-the-art engine combustion model including chemical kinetics with a total of 42 model parameters with their corresponding uncertainties.

2 Model development

Conventionally, the concept of a *model* is usually considered as a set mathematic equations which describe a physical system or process, however these descriptions are usually incomplete at some level and require the adoption of "optimizable" parameters. Given that these parameters are coupled to the experimental data adopted in their formation, here a *model* is redefined to include the mathematic equations as well as the experimental dataset used for parametric optimization [4].

Based on our definition, a *model* can be separated into three sub-components.

1. *Data models*: Which outline the structure that data is stored in.
2. *Instrumental models*: Which are used to translate an observation into a useful metric, for example a thermocouple translates a measurement of capacitance via a correlation into a measurement in standard units e.g. ^{o}C.

3. *Application models*: Which are the mathematic equations which describe the physical process which occur in the *"real world"*.

Whether unknown, or known to be in a particular range, these parameters must be obtained from carrying out an optimization and validation phase with respect to experiment observations, which ideally would be using a comprehensive and state of the art database. Hence to apply all of these concepts to an automated engine development process, three major developments are required, (1) a standardized *data model* for storing and sharing experimental and model data, (2) for *application models* to be extended to include parametric uncertainties, and (3) for the adopted optimization routine to include experimental and parametric uncertainty.

The sections which follow detail the methods employed in applying these concepts to the engine development process.

3 A data model: engineRDF

The eXtensible Markup Language (*XML*) is used as the fundamental code of the engine Markup Language (*engineML*) [5]. The structure is fully extensible, an open standard and is platform independent making it potentially timeless and thus ideal for Process Informatics approaches. In addition, an *XML schema* can be adopted to ensure consistency between files created from multiple users and multiple programs which is important in creating standardization for large collaborative research activities such as engine development.

The *engineML* data model is separated into *General data* (independent of operating point) and *Case data* (dependant on the operating point), each are then divided into *Basic*, *Intake*, *Injection*, *Fuel*, *Cylinder* and *Exhaust* for simple referencing. The extensibility of the structure means that if the database does not contain a component that the user requires, it can be added without compromising the structure of the infrastructure (the additional data would also be compatible with any legacy software). Table 1 shows data and metadata which are defined in an example *engineML* property entry. The design of a *property entry* is flexible enough to contain a wide range of engine data. A sample *engineML* property is presented in Figure 1 according to the data structure shown in Table 1.

For data to be useful in the long term, it is critical to properly define the apparatus and measurement devices as this ensures a comprehensive record of the experiment is held with the experimental measurements. Furthermore this information is of great importance for model developments which include error and uncertainty propagation as described in the example in this paper.

Often a large number of automatically measured data are categorized or grouped into sets of the same type and each data set is normally stored into separate *XML* files, i.e. *engineML*. However, in order to use the formatted *XML* data effectively, one must understand its representation or the corresponding *schema*. Naturally it is preferable to access these data without learning the full knowledge of an *XML* based representation, which can be done via the adoption of *Semantic Web* technologies, such as *RDF* (Resource Description Framework).

In this work, *engineML* data are transformed in such ways that each useful data resource is uniquely identified by *URI* (Uniform Resource Identification) and these are related to each other using a proper *RDF-statement* as shown in Figure 2. Firstly, in order to relate these data to one another, the semantic relationship of the data resource must be defined. The *datatypes* and relationships (predicate) for *engineRDF* are defined in Table 2 and Figure 2 respectively. The *URI* pattern shown in Figure 3 enables users to uniquely identify each resource whilst containing the full information about its higher level resources.

The transformation of *engineML* into *engineRDF* turns *legacy data* into a web network of engine data which allows everyone, including computer resources, to understand these data through their relationships rather than their representation. Since each *engineRDF* contains unique information, this was considered more robust than equivalent *XML* based approaches, and thus an improvement upon our original *engineML* structure [5]. In this work we have adopted a *triplestore* database engine, an example is *openRDF-sesame* which is a *Java-based* with support for *RDF Schema* inferencing and querying. It supports both local and remote through *http* protocol allowing data to be exchanged globally over the internet.

A data repository has been populated with a comprehensive set of state-of-the-art experimental data supplied by the *Lund Institut of Technology* [6–9], at present this data can be queried and visualized via the *Cambridge University* web pages [10] enabling engineers from all over the world to access these data for their own model development purposes.

```
<property
    variable_name="Intake valve diameter"
    short_name="Int.Dia"
    detailed_description="Intake valve diameter"
    measurement_device="unknown"
    measurement_location="NA"
    data_type="constant"
    data_structure="point"
    unit="mm"
    unit_reference="none"
    unit_type="length">
    <value>50.0</value>
    <uncertainty>0.00</uncertainty>
</property>
```

Figure 1: *Example of engineML data model: Intake valve diameter property*

Table 1: *engineML properties*

XML tag or name	*XML syntax* type	Description
engineml:variable_name	xs:attribute	Name of data
engineml:short_name	xs:attribute	Short name of data
engineml:detailed_description	xs:attribute	Description of the data
engineml:measurement_device	xs:attribute	Equipment used to take data
engineml:measurement_location	xs:attribute	Measurement location
engineml:unit	xs:attribute	Units (e.g. degrees)
engineml:unit_reference	xs:attribute	Relative unit (e.g. bTDC or aTDC)
engineml:unit_type	xs:attribute	Data type (e.g. a crank angle)
engineml:data_structure	xs:attribute	Data structure
engineml:value	xs:element	Value of data
engineml:profile	xs:element	Profile of data (e.g. x,y)
engineml:uncertainty	xs:element	Uncertainty of data

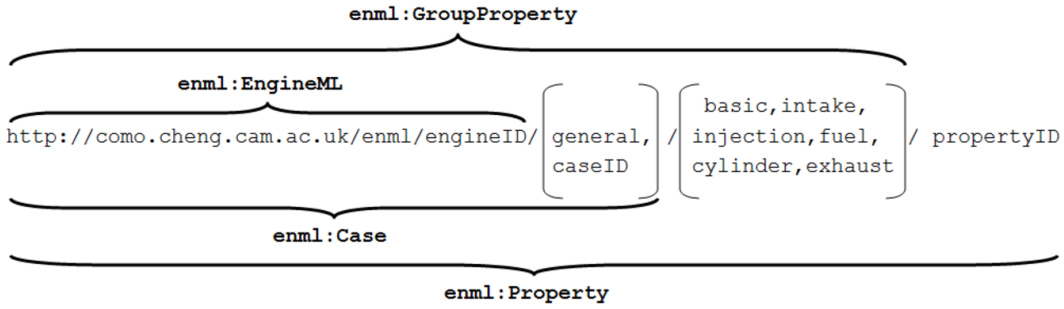

Figure 2: *URI of engineRDF datatype*

4 Optimization

The optimization consists of two main stages: (1) Parameter optimization done by evaluating the full model, achieved in two steps, and (2) Parameter and model response uncertainty estimation done by evaluating linear response surfaces.

The parameter vector $\mathbf{x}$ is defined as:

$$\mathbf{x} = (\mathbf{E}, \mathbf{R}) \,, \tag{1}$$

where $\mathbf{E}$ and $\mathbf{R}$ are as described in Table 5.

Asthe first step of the parameter optimization, data points in the 42-dimensional parameter space were generated using Halton [11] low discrepancy sequences. The model was evaluated at these points and the objective function Φ_1:

$$\Phi_1(\mathbf{x}) = \sum_{i=1}^{N} \sum_{j=1}^{M_i} \left(\frac{\eta_{ij}^{\text{exp}} - \eta_{ij}(\mathbf{x})}{\sigma_{ij}^{\text{exp}}} \right)^2 \tag{2}$$

determined, where N is the number of operating points and M_i is the number of experimental data points from the i^{th} operating point. η_{ij}^{exp} are the experimental values of: ignition delay crank angle; peak pressure; peak pressure crank angle and the pressures closest

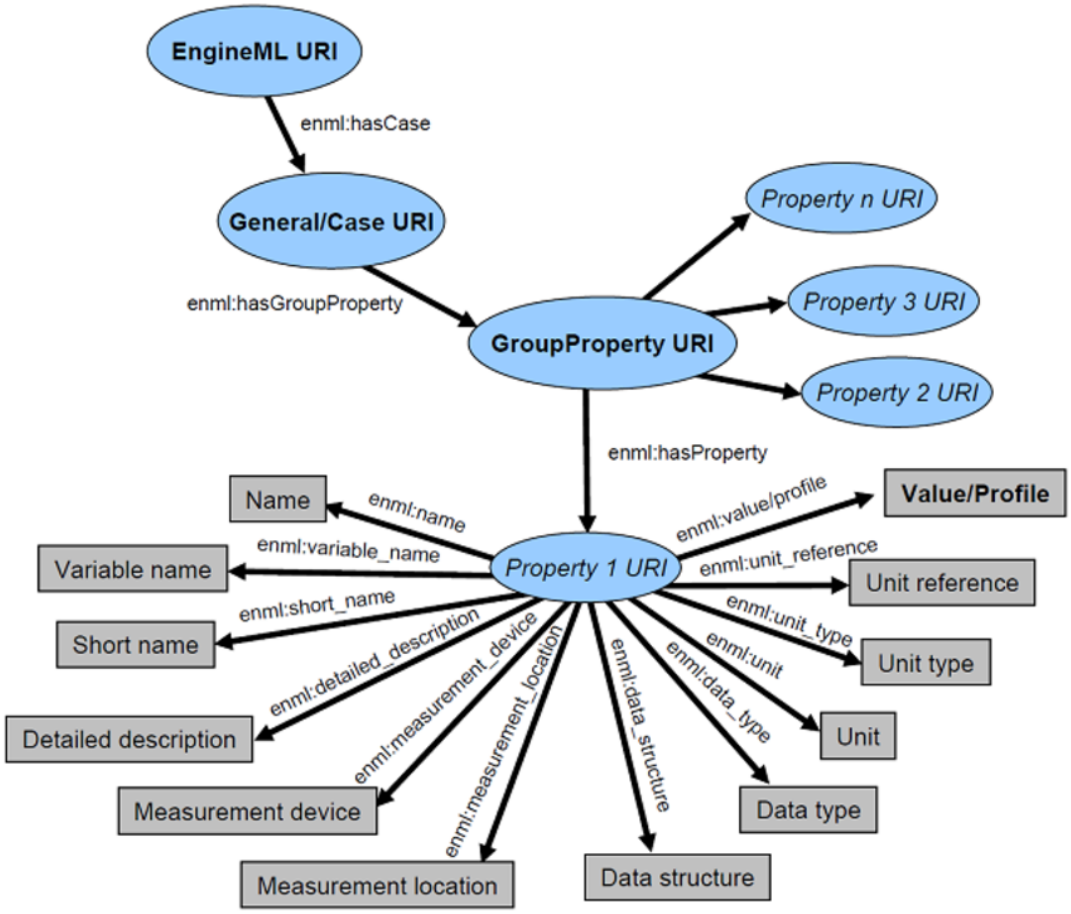

Figure 3: *The engineRDF predicate which relate the subject to the object*

to increments of 5 bar (these pressure points can be seen in Figure 4). $\eta_{ij}(\mathbf{x})$ are the model responses for: ignition delay crank angle; peak pressure; peak pressure crank angle and the pressure at each crank angle at which the experimental pressures were sampled. The set of parameters $\mathbf{x}_1^*$ that minimizes the objective function Φ_1:

$$\mathbf{x}^* = \underset{\mathbf{x}}{\operatorname{argmin}} \{\Phi_1(\mathbf{x})\} \tag{3}$$

has been determined.

As the second step of parameter optimization the model has been optimized using the Levenberg-Marquardt algorithm taking $\mathbf{x}_1^*$ as the starting point. A new set of parameters $\mathbf{x}_2^*$ have been determined that minimized Φ_1 further.

As the final stage a linear response surface optimization has been performed around the point $\mathbf{x}_2^*$ and the uncertainties in the parameters and in the model response have been estimated. This methodology has been proposed by Sheen et al. [12] and used by Braumann et al. [13, 14] to optimize a granulation model and a system level soot model [5].

It is assumed that the free parameters $\mathbf{x}$ are Gaussian distributed and have a mean $\mathbf{x}_0$ and

Table 2: *engineRDF datatype*

datatype	Description
enml:EngineML	An *RDF* type which represents an *engineML* document.
enml:Case	An *RDF* type which represents a case of the *engineML*. The case can be general case data or operating-point data.
enml:GroupProperty	An *RDF type* which represents property group within the case, i.e. Basic, Intake, Injection, Fuel, Cylinder and Exhaust.
enml:Property	An *RDF type* which represents property in *engineML*.

a standard deviation $\mathbf{c}$:

$$\mathbf{x} = \mathbf{x_0} + \mathbf{c}\,\xi\,, \tag{4}$$

where ξ is normally distributed.

It is convenient to normalize the free parameters $\mathbf{x}$ to $\tilde{\mathbf{x}}$ and $\mathbf{c}$ to $\tilde{\mathbf{c}}$, where $\tilde{x}_k \in [-1, 1]$ and $\tilde{c}_k \in [0, 2]$, $k = 1, 2, \ldots, 42$. The model responses $\eta_{ij}(\mathbf{x})$ have been approximated by linear response surfaces, $\mu_{ij}(\tilde{\mathbf{x}})$:

$$\eta(\mathbf{x}) \approx \mu(\tilde{\mathbf{x}}) = \beta_0 + \sum_{k=1}^{42} \beta_k\,\tilde{x}_k\,, \tag{5}$$

where the i and j indices have been suppressed, around the point $\mathbf{x}_2^*$. The coefficients β_0 and β_k have been calculated using finite differences:

$$\beta_0 = \eta(\mathbf{x}_2^*)\,, \tag{6}$$

$$\beta_k = \frac{\eta(x_{2,1}^*, \ldots, (x_{2,k}^* + 1), \ldots, x_{2,42}^*) - \eta(x_{2,1}^*, \ldots, (x_{2,k}^* - 1), \ldots, x_{2,42}^*)}{2}. \tag{7}$$

The variance $\sigma^2(\tilde{\mathbf{c}})$ of the model response can be written as:

$$\sigma^2(\tilde{\mathbf{c}}) = \sum_{k=1}^{42} \left(\beta_k \tilde{c}_k\right)^2. \tag{8}$$

The objective function is based on the principle of moment matching to reduce bias and limit the parametric uncertainties to the experimental error:

$$\Phi_2(\tilde{\mathbf{x}}_0, \tilde{\mathbf{c}}) = \sum_{i=1}^{N} \sum_{j=1}^{M_i} \left(\frac{\eta_{ij}^{\text{exp}} - \mu_{ij}(\tilde{\mathbf{x}}_0)}{\sigma_{ij}^{\text{exp}}} \right)^2 + \left(\frac{\sigma_{ij}^{\text{exp}} - \sigma_{ij}(\tilde{\mathbf{c}})}{\sigma_{ij}^{\text{exp}}} \right)^2 . \tag{9}$$

Minimizing the objective function $\Phi_2(\tilde{\mathbf{x}})$ using the Levenberg-Marquardt routine leads to the optimal set of model parameters and their associated errors:

$$(\tilde{\mathbf{x}}_0^*, \tilde{\mathbf{c}}^*) = \underset{\tilde{\mathbf{x}}_0,\, \tilde{\mathbf{c}}}{\text{argmin}} \left\{ \Phi_2(\tilde{\mathbf{x}}_0, \tilde{\mathbf{c}}) \right\} . \tag{10}$$

5 Application to an in-cylinder IC engine model

5.1 Application model

The methodology outlined above was applied to optimize an engine combustion model against the engine experimental data stored in the repository. The underlying engine model was the Stochastic Reactor Model (SRM) [15], in the past the SRM has been successfully employed in a number of studies of port fuel injected HCCI combustion [16], surrogate fuel blends [17], single early direct injection HCCI [18], dual injection HCCI [19], multi-cycle transient simulation and control [20], soot formation [21], and has been coupled to the Computational Fluid Dynamics (CFD) code KIVA [22]. Further details of the model can be obtained from these studies however in summary, the SRM is able to simulate the internal mixing and chemical processes in the combustion chamber, along with heat transfer to the cylinder walls. It is the preferred tool for modeling HCCI combustion than conventional fully homogeneous models as it allows for temperature and mixture inhomogeneities which are important in smoothing out the observed heat release rates.

The fuel oxidation chemical kinetic models have a large number of parameters, often in the thousands [23] requiring serious computational cost, however given that this is an example of the methodology and to keep it industrially relevant, a skeletal iso-octane/n-heptane oxidation mechanism developed by the *Nissan Motor Company* containing 33 species and 38 reactions was adopted [24]. Importantly, the infrastructure of carrying out the optimization with the employed model is identical to that of a semi-detail, detailed or comprehensive chemical kinetic mechanism and engine model.

The SRM code was manipulated to read directly from the *engineRDF* files, enabling rapid and consistent model initialization directly from experimental data. However, not all data was immediately accessible for example, the SRM is an in-cylinder model and thus only solved between inlet valve closure and exhaust valve opening, however in practice, measurements for initial mixture pressure and temperature at inlet valve closure often come via estimation based on the measurements obtained in the intake manifold. Here we imposed a simple engine breathing model, via a single multiplier upon the manifold pressure and temperature measurements to generate a relevant initial mixture state.

5.2 Data model

Details of the data adopted for the optimization to set up the initial parameters are outlined in Table 3 and 4. The employed data were those relevant to pure iso-octane fuel blends, with the engine operated in HCCI operating mode. In this example, seven operating points have been included however, the infrastructure enables as many as required to be adopted.

Listed in Table 5 are a list of the initial model parameters and their corresponding one standard deviation uncertainty for the model parameters. Initial engine parameters were obtained directly from the experimental data stored in the *engineRDF* webportal, with typical expected uncertainty bands employed. The SRM engine model was adopted with

five stochastic particles and with an initial stochastic heat transfer parameter of 2000. The initial reaction rates adopted in the fuel model were obtained from [24], however an uncertainty was only employed for the pre-exponential term, A with the other fuel model parameters assumed to have no uncertainty. An optimization was carried out by varying these parameters minimizing the objective function (2) , within their uncertainty bounds with respect to the ignition delay time, peak pressure and the in-cylinder pressure profile (at 5 bar increments), experimental errors of 3 bar, 2 CAD and 3 bar were adopted respectively. The first objective function, Equation (2), was calculated from the model response at over 200 points during the Halton sequencing step taking 3 hours, the Levenberg-Marquardt optimization evaluating the model response took 2 hours and the response surface was determined within 3 hours on a standard desktop PC.

Table 3: *The data repository employed for the optimization*

Data type	Description	Reference
Reaction rate parameters	Obtained via comparisons with engine data and ignition delay times	[24]
Experimental engine data	HCCI operating mode Stroke = 140mm Bore =120.65mm Con-rod length=260mm CR=17.0 IVC=-167.0^{o}aTDC EVO=141.0^{o}aTDC	[8]

Table 4: *The engine operating points*

Case number	Manifold pressure [bar]	Manifold temperature [K]	Equivalence ratio [-]	Internal EGR fraction [-]	Engine Speed [RPM]
1	0.967	367.2	0.392	0.1	697
2	0.970	376.2	0.337	0.1	696
3	0.971	385.0	0.288	0.1	698
4	0.970	396.4	0.252	0.1	696
5	0.971	407.5	0.225	0.1	696
6	0.952	386.5	0.390	0.1	995
7	0.935	393.9	0.330	0.1	995

5.3 Results

The final results of the optimization are presented in Table 5. In all cases other than for the stochastic heat transfer parameter, a new set of model parameters and a reduced set of model uncertainties were obtained including a reduction of the uncertainties on the reaction rates, here shown as a mean value.

The results of the computations in terms of pressure-crank angle are presented in Figure 4. The experimental data are shown, where each point represents those which were included in the objective function. The solid black line represents the result of the initial set of parameters, where in all cases the ignition was early compared to the experiment, with higher pressures from -30^{o}aTDC to TDC.

The result of the minimization of first objective function yielded a new set of model parameters which best fitted these experimental data, the results of these parameters are also presented in Figure 4 as a broken black line and have been made available in the supplementary material. In all cases compression and expansion were computed well, with the main heat release generally computed a little late, however there is a significant improvement compared to the results obtained with the original set of model parameters. Neither Cases 6 or 7, which were obtained for an engine speed of 995 RPM, achieved the peak pressure, however this may well be associated with the number of particles and the stochastic heat transfer parameter tending to zero.

The corresponding initial model uncertainty is also presented as the dark grey shaded regions, whilst these are often based on the initial values, these can often be arbitrary as shown in Table 5, however they have been constrained to what might be expected as a reasonable deviation. During compression, the errors associated with the initial pressure, temperature and compression ratio are smaller than the thickness of the line, however once the heat release begins, typically at around -10^{o}aTDC, the influence of the chemistry becomes more influential and thus the uncertainty upon those parameters contained in the fuel oxidation model become more significant. In all cases, the largest uncertainties are noted in those regimes where the chemical kinetics are most active. However in some cases, at the maximum and minimum limits, the response of the model appears disjointed, this is most likely to be associated with the adoption of a linear response surface to represent what is a non-linear problem, as such these aspects would be expected to be most prominent when extrapolated to the limits.

The result of the minimization of the second objective function yields a final set of uncertainties, which are presented as the light grey region in Figure 4. Firstly (whilst not clear from the figure) the uncertainty of the model during the compression phase reduced due to the reduction of the uncertainty on the engine parameters E1 to E4 shown in Table 5. However the main reduction in the uncertainty was in the regime dominated by the chemical kinetic parameters, R1 to R38. Here the uncertainty was reduced from up to 20 bar to around 3 bar, typically this uncertainty was largest at around TDC and then reduced during the expansion stroke as the influence of the kinetics reduced and those associated with thermodynamic expansion began to dominate.

Between the intake manifold and IVC, it would be expected that the mixture temperature would increase due to processes such as wall to gas heat transfer and mixing with trapped exhaust gases, however during the optimization the final multiplier on the initial temperature parameter was less than 1.0 suggesting that the in-cylinder initial temperature is lower than that in the manifold. This is unlikely hence it is expected that other parameters such as the compression ratio and the reaction rates are compensating for this in order to minimize the objective function with respect to these experiments. Hence an improved initial estimate of this parameter may well yield an improved result.

The adoption of only five stochastic particles has reduced computational times at the expense of dealing with the inherent inhomogeneities noted in HCCI engines, for example 100 stochastic particles have been adopted for carrying out these similar simulations on this same engine [17]. With the adoption of only five particles, it is likely that the stochastic heat transfer parameter could not find an optimum and with so few particles it has little impact on the final result. The natural next step for this study would be to increase the number of particles and to include more experimental data to seek to reduce the uncertainties in the chemical kinetics parameters further.

Table 5: *Normalized initial and final model parameters with their corresponding uncertainties*

Parameter	Description	Initial value	Initial uncertainty	Final value	Final uncertainty
E1	Compression ratio	1	0.2	0.985	0.002
E2	Initial pressure multiplier	1	0.2	0.955	0.021
E3	Initial temperature multiplier	1	0.2	0.917	0.012
E4	Stochastic heat transfer parameter	1	2	0	2
R1 ... R38	Forward reaction rate pre-exponents, $A_{R1...R38}$	1	2	-	0.41

6 Discussion

The example demonstrates the power of automating data storage, retrieval and model optimization to reduce the man-hours required to tune models to large experimental datasets and thus retain the *knowledge* contained within them. Furthermore, the model robustness can be enhanced by reducing known uncertainties with respect to experiments, these can be used to identify those experimental data which can be modeled with confidence and also those aspects of the model which need improvement. This enables senior engineers to distribute resources appropriately to then go on and solve model development problems more effectively.

The web portal enables all engineers to have access to a comprehensive engine data repository. Researchers are encouraged to upload their experimental data to the repository, this ensures that these data are stored securely in a consistent format for future research activities and facilitating knowledge transfer between research groups. The most significant advantage will is for the modeling community as a whole who now have, for the first time a data repository of well marked-up experimental data for automated model operation and optimization.

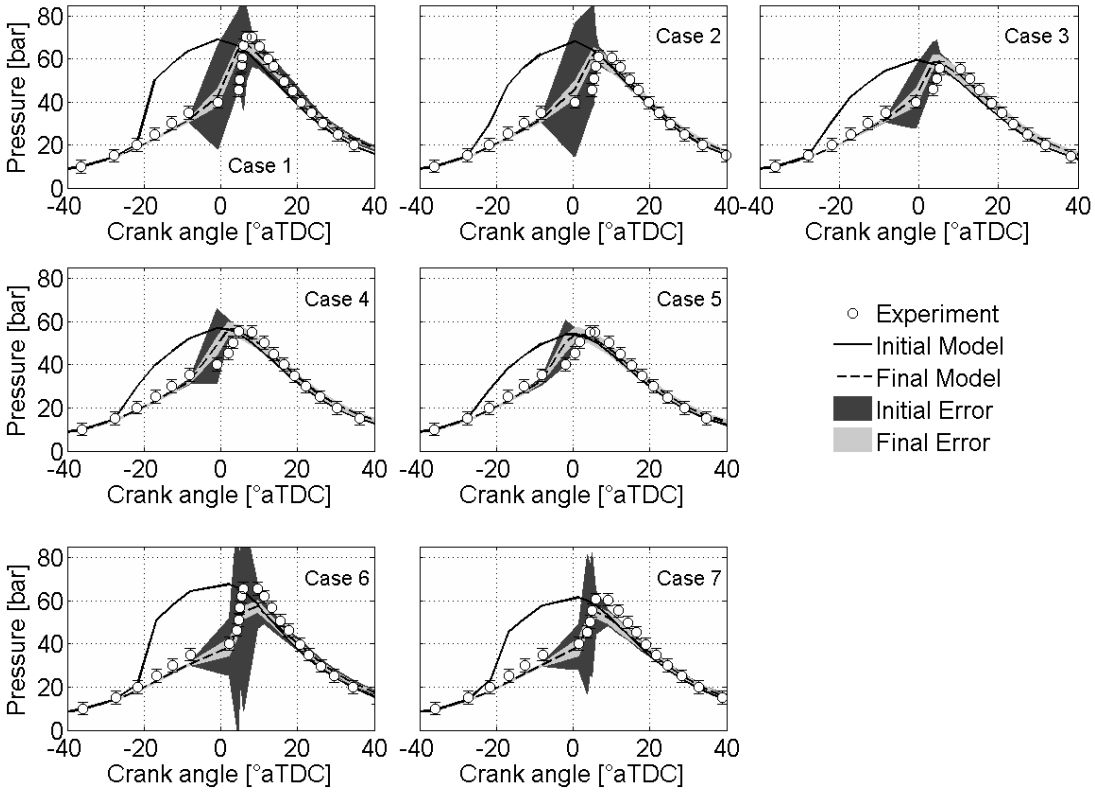

Figure 4: *In-cylinder pressure-crank angle diagrams for all cases.*

7 Conclusions

The *engineML data model* used for storing engine based experimental data has been extended to an *engineRDF* format for improved searching and querying. A web portal for storage, searching and visualization of engine data has been developed for engineers to extend a repository of shared engine data for improved knowledge transfer and automated model development.

Using the described methodology, an engine model containing more than forty input parameters has been systematically optimized against engine experimental data held in the data repository. Adoption of the methodology has demonstrated that engine model parametric uncertainties can be reduced with respect to experiments and highlighted those aspects of the model which are most sensitive these uncertainties.

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