

Software to Calculate Reaction Rates in Clean Energy Fuels Using High-level Programming Language

Reverse Engineered from Industry Software.

Goal: To simplify software to make easier to understand and facilitate collaborate, and to create an educational tool to promote learning.

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Software Flow Chart

Read fuel mechanism,
stores values into
intermediate variables

Mechanism file includes NASA polynomials for thermodynamic data, where 7 numbers are used to calculate quantities such as specific heat, enthalpy, entropy, etc.

$$\frac{c_p}{R_u} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

The most basic type of reaction is a modified arrhenius equation of the following form.

$$k_f = A * \left(\frac{T}{T_0} \right)^B * \exp \left(\frac{E_A}{R_u T} \right)$$

It uses 3 coefficients, A the pre-exponential factor, B the temperature exponent, and E_A the activation energy

This is how the reaction appears in the mechanism file

O+H2<=>H+OH 3.870E+04 2.700 6260.00

This means
the reaction
is both
forward and
reverse

A the pre-
exponential
factor
Unit depends
on reaction

B the
temperature
exponent
Dimensionless

E_A the
activation
energy
Units of
Calorie

Print code to calculate
reaction rates, can stand
alone as it's own program

This is called the "create hardcode" step because the code generated is specifically for a certain fuel, for example methane (CH4) or hydrogen (H2). This code will be available for free download under the GNU General Public License at CombustionHelp.com

This part of the code is very easy to understand, more so than the industry code, better for learning/ collaborating/experimenting.

Here is code of the same O+H2<=>H+OH reaction

```
kf=kfarray(3);  
fwdk(3)=kf*Y(1)*Y(3);  
Kc=exp( -(+g(1)*-1+g(2)*1+g(3)*-1+g(5)*1) / T );  
revk(3)=kf/Kc*Y(2)*Y(5);
```

Y(1) is the mole concentration of $\frac{mol}{cm^3}$
hydrogen (H2), Units of

fwdk(3) is the forward reaction rate $\frac{mol}{cm^3 * sec}$
of the 3rd reaction, Units of

Reactor simulations call
reaction rate functions

How to call function to get molar production rate

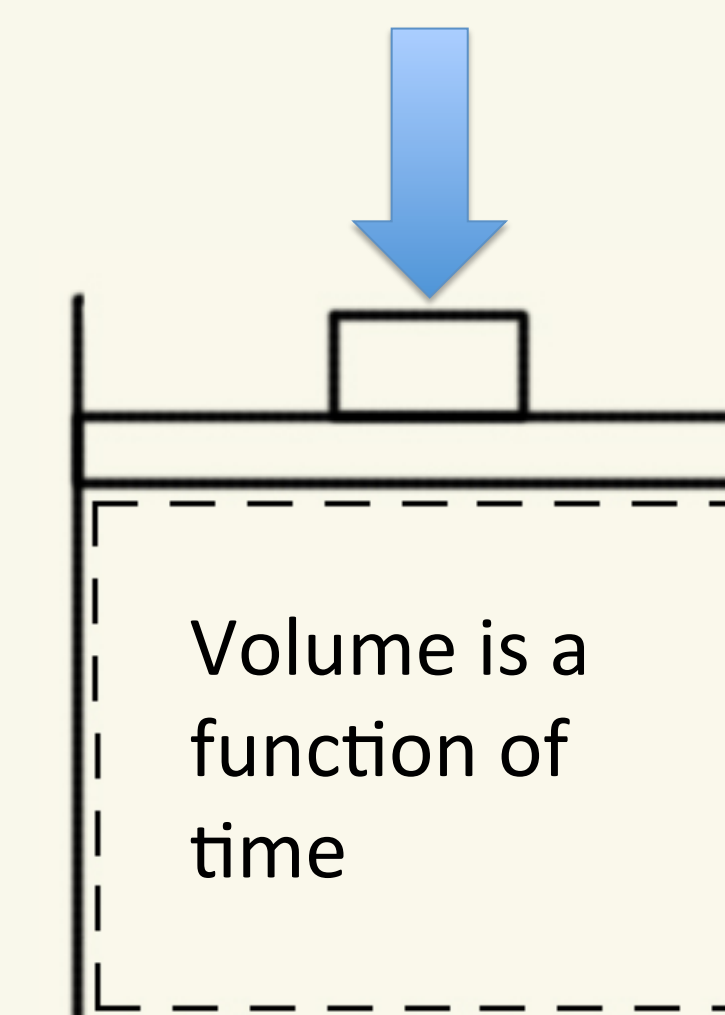
Vector of molar production rate
Units of $\frac{mol}{cm^3 * sec}$

$w_{dot} = getwc(C, T)$

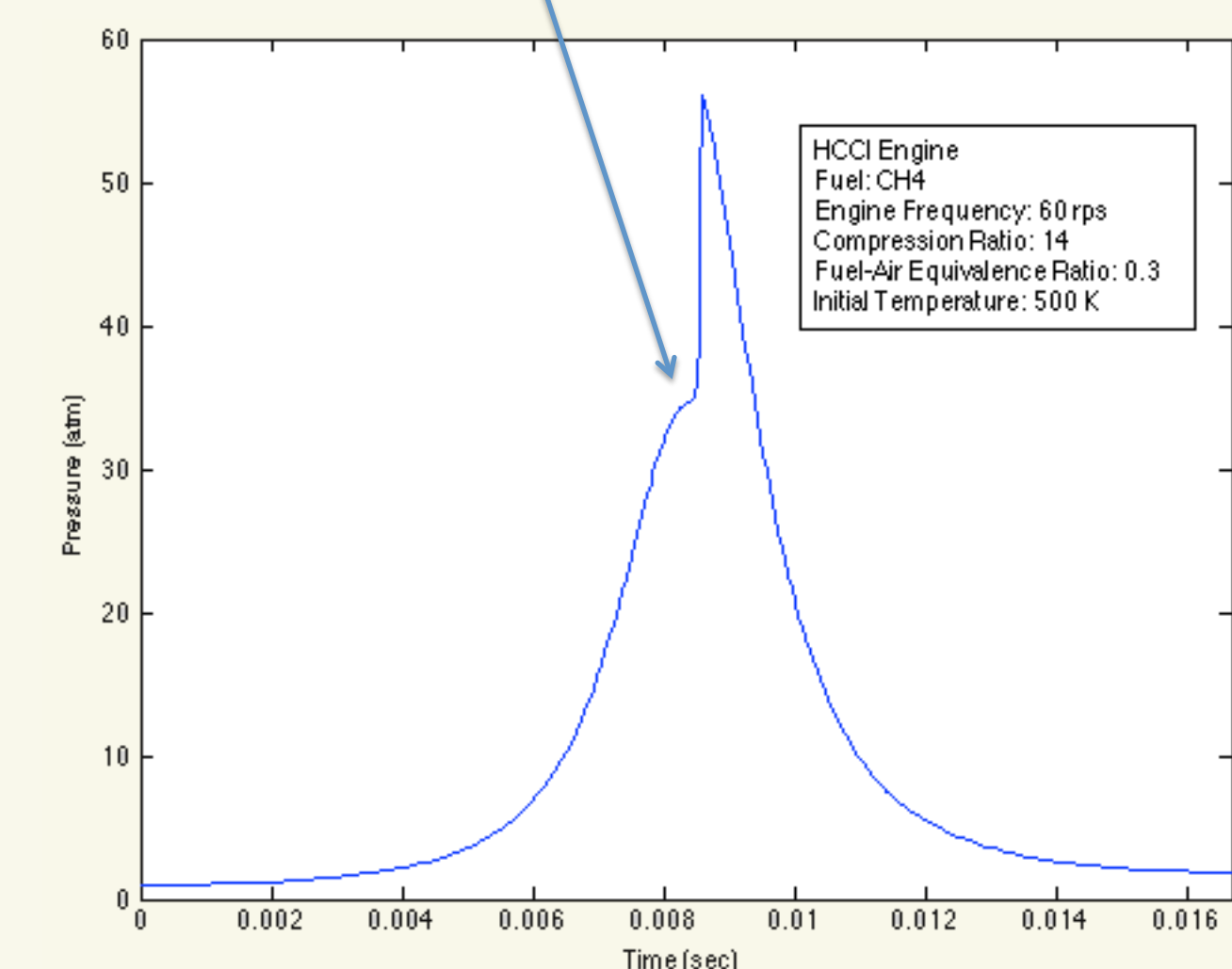
Temperature Units of Kelvin

Vector of molar concentration
Units of $\frac{mol}{cm^3}$

HCCI engine – Premixed fuel and air injected into cylinder, ignition occurs from compression just as in diesel engine



Mixture compressed until it ignites



HCCI Engine
Fuel: CH4
Engine Frequency: 60 rps
Compression Ratio: 14
Fuel-Air Equivalence Ratio: 0.3
Initial Temperature: 500 K

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