# MReaDy manual

*Dr. César Mogo**
*University of Algarve*
*Version 1*

**Abstract**

MReaDy is a program for studying reactive dynamic systems using a global potential energy surface built from previously existing potential energy surfaces corresponding to each of the most important elementary reactions present in the system. This manual describes and points out standard working procedures for the MReaDy program and its several forks. It is a continuous effort towards a final optimal form that will never be attained.

# Contents

---
* cfmogo@ualg.pt

# 1 Introduction

MReaDy (Multiprocess Reaction Dynamics program) is a program for studying reactive dynamic systems using a global potential energy surface (gPES).

Potential Energy Surfaces (PES), based on *ab initio* calculations, is a powerful tool to study the rate of elementary reactions and their dynamics, being useful to compute state-to-state rate constants. In a more complex mechanism, we will be in the presence of different and simultaneous elementary reactions, corresponding to all the possible reactive and non-reactive collisions between the species present and leading to the respective products. Attempting to build a traditional PES for such a system easily becomes impossible. To circumvent this problem, a global Potential Energy Surface (gPES) can be defined by integrating various PESs, each representing an elementary reaction expected to play a role in the chemical process. MReaDy is built in such a way and performs reactive dynamic calculations based on such gPES.

This manual intends to present MReaDy and how to use it. There are several versions of MReaDy, but this manual will target the MReaDy Base version since most of its working principles are common to the remaining versions.

How to reference MReaDy:

## 1.1 MReaDy versions

Its first intent of MReaDy was to simulate hydrogen combustion, but it later forked into several versions:

MReaDy Base
: A version including all available PES, aiming to simulate hydrogen combustion up to molecules with four atoms[1].

MReaDy OH
: A version including all available PES, aiming to simulate hydrogen combustion up to molecules with four atoms but where the formation and destruction of OH radicals are followed.

MReaDy CNT
: MReaDy has been adapted to study the combustion of molecular hydrogen confined in SWCNTs under varying nanotube diameter, gas pressure, and temperature conditions. This adaptation allows for comprehensively exploring the combustion process within the nanotube environment[2].

MReaDy HO2
: The program starts with reactants at desired initial conditions and removes the reaction products once they are formed. To maintain constant energy and concentration of the reactants, new reactants replace the removed species with the same total energy. By employing this approach, MReaDy replaces the traditional method of treating each collision independently by calculating a bulk of trajectories that can interact, thereby enabling a focus on the collisional stabilization process. Specifically, only the collision between an H atom and an $O_2$ diatomic can produce a new molecule. In contrast, the remaining collisions proceed through non-reactive PESs, and this way, taking into account energy transfer between the colliders.[3, 4].

## 2 Working blocks

The MReaDy code comprises several blocks and files, as Figure 1 shows. Below is the description of the main components.

**parameters.f90** : Where the simulations' initial physical and chemical conditions are set. It includes temperature, volume, and composition, among other working parameters such as the number of steps, printing, backup, etc.

**generate_*.f90** : Generation files where the several molecules' generation is set.

**verlet_alg.f90** : Algorithm, the center of the program.

**potential_total.f90** : gPES calculation.

**agrupa.f90** and **desagrupa.f90** : Forming and Binging molecules.

**write_geom.f90** : Output formats and commands code.

**geo*.xyz** : Cartesian coordinates and velocities for each atom and the system's total potential and kinetic energy. Data is written on the file according to printing time.

**time_changes*.cvs** : Where information about the chemical composition is written whenever a molecule is formed or destroyed.

**\*.bk** : Backup files needed for restarting the program.

Main variables:

*group* matrix : Where each molecule's composition information, including colliding partner, is saved.

MReaDy's main feature is to treat the global mixture as a unique global potential energy surface built from the potential energy surfaces of the different present species. Each atom is in a defined electronic state in a particular molecular system. The potential acting on each atom is the sum of the interactions within its molecular system and the long-range interactions with all the remaining atoms. These calculations are accomplished in the "Compute potential and derivatives" block seen in Figure 1.
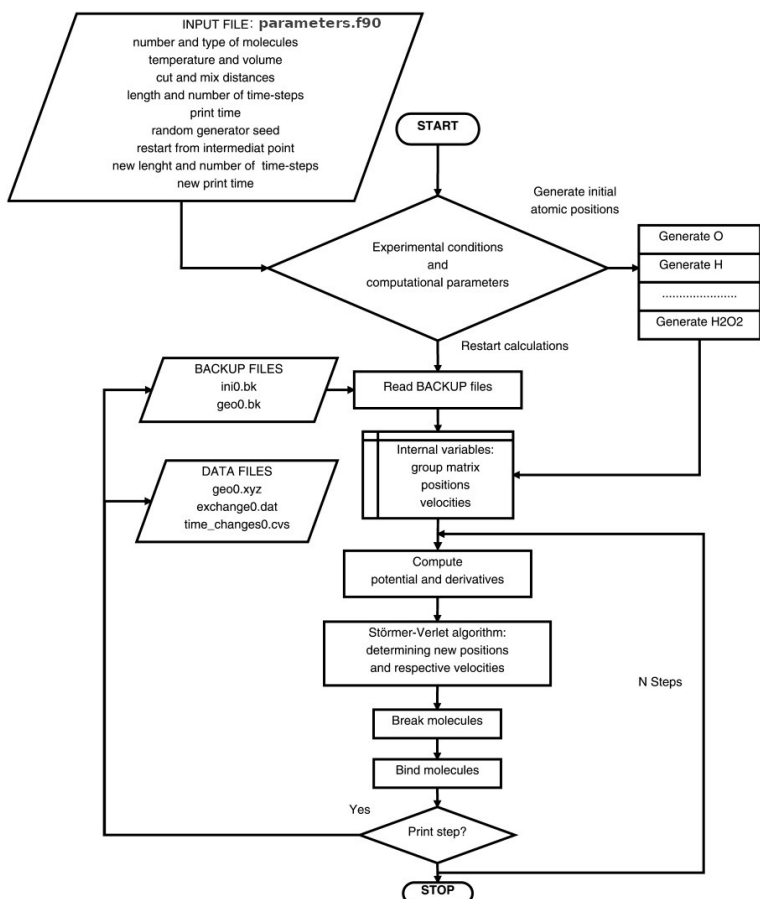
Figure 1: MReaDy flow chart

By molecular system, we mean any group of atoms for which a PES is available. Each PES is identified with an integer called system ID for programming purposes. Similarly, each atom has an atom ID. All the relevant information necessary to define the gPES is kept on an integer matrix, named *group*, which records the number of atoms, the molecular system ID, the atoms ID, and, when participating in a non-reactive collision, the system ID of the other partner.

MReaDy was built modularly so that any PES can be replaced or new ones be further implemented. MReaDy has 18 PESs quoted on Tab. 1, covering the main collisions, up to four atoms, in which reaction can occur. MReaDy is not limited to four atoms PESs, but accurate full-dimensional PESs for larger systems become increasingly difficult to produce.

Table 1: PES used in MReaDy program

| Diatomics | Triatomics | Tetra-atomics |
|---|---|---|
| $H_2(^1\Sigma)$ | $H_3(^2)$[19] | $H_4(^1B_1)$[20] |
| $H_2(^3\Sigma)$ | $H_2O(\tilde{X}^1A')$[21] | $H_3O$ [22] |
| $HO(^2\Pi)$ | $H_2O(^3A'')$[23] | $H_2O_2(^1A)$[24] |
| $HO(^4\Sigma)$ | $HO_2(^2A'')$[25] | $H_2O_2(^3A)$[26] |
| $O_2(^3\Sigma)$ | $O_3(^1A_1)$[27] | $HO_3(^2A)$[28] |
| $O_2(^1\Delta)$ | | $O_4(^3A)$[29] |
| $O_2(^5\Pi)$ | | |

To compute the long-range interactions, we use atom-atom potentials

Table 2: Representation of the several chemical combinations predicted in MReaDy. Currently, the maximum number of atoms permitted per molecule is four.

| | O($^3$P) | O($^1$D) | H($^2$S) | H$_2$($^1\Sigma$) | O$_2$ ($^3\Sigma$) | O$_2$($^1\Delta$) | HO($^2\Pi$) |
|---|---|---|---|---|---|---|---|
| O($^3$P) | 3/81 O$_2$($^3\Sigma$) / 78/81 n.r. | | | | | | |
| O($^1$D) | n.r. | n.r. | | | | | |
| H($^2$S) | 2/3 HO($^4$) / 2/9 HO($^2\Pi$) / 1/9 n.r. | n.r. | 1/4 H$_2$($^1\Sigma$) / 3/4 H$_2$($^3\Sigma$) | | | | |
| H$_2$($^1\Sigma$) | 1/3 H$_2$O($^3$A") / 2/3 n.r. | 1/5 H$_2$O($\tilde{X}^1$A') / 4/5 n.r. | H$_3$($^2$) | H$_4$($^1$B$_1$) | | | |
| O$_2$ ($^3\Sigma$) | 1/9 O$_3$($^1$A$_1$) / 8/9 n.r. | n.r. | 1/3 HO$_2$($^2$A") / 2/3 n.r. | H$_2$O$_2$($^3$A) | 1/3 O$_4$($^3$A) / 2/3 n.r. | n.r. | |
| O$_2$($^1\Delta$) | n.r. | n.r. | n.r. | H$_2$O$_2$($^1$A) | n.r. | n.r. | n.r. |
| HO($^2\Pi$) | 1/3 HO$_2$($^2$A") / 2/3 n.r. | n.r. | 1/4 H$_2$O($\tilde{X}^1$A') / 3/4 n.r. | H$_3$O | HO$_3$($^2$A) | n.r. | 1/4 H$_2$O$_2$($^1$A) / 3/4 H$_2$O$_2$($^3$A) |
| HO$_2$($^2$A") | 1/3 HO$_3$($^2$A) / 2/3 n.r. | n.r. | 1/4 H$_2$O$_2$($^1$A) / 3/4 H$_2$O$_2$($^3$A) | | | | |
| H$_2$O($\tilde{X}^1$A') | H$_2$O$_2$($^3$A) | 1/5 H$_2$O$_2$($^1$A) / 4/5 n.r. | H$_3$O($^2$) | | | | |
| H$_2$O($^3$A") | 1/9 H$_2$O$_2$($^1$A) / 8/9 n.r. | n.r. | 1/3 H$_3$O($^2$) / 2/3 n.r. | | | | |
| O$_3$($^1$A$_1$) | 1/3 O$_4$($^3$A) / 2/3 n.r. | n.r. | HO$_3$($^2$A) | | | | |
| H$_3$($^2$) | 1/3 H$_3$O($^2$) / 2/3 n.r. | n.r. | 1/4 H$_4$($^1$B$_1$) / 3/4 n.r. | | | | |

built from accurate *ab initio* calculations for the interaction with the highest spin state compatible with the ground state of the atoms, according to the Wigner-Witmer spin and symmetry correlation rules, namely H$_2$($^3\Sigma$), O$_2$($^5\Pi$) and HO($^4\Sigma$). This warrants a non-bonding interaction. A repulsive short-range exponential term and a long-range van der Walls attraction damped at short distances describe the diatomic potentials.

## 2.1 Breaking and creating bonds

To define the molecular systems present in the mixture, at each integration step, the MReaDy program analyzes the inter-atomic distances and, according to the user's defined breaking and forming distances, determines which molecular systems are broken or newly formed, updating the matrix *group*.

The first step, the breaking procedure, is carried out similarly to the one used by quasi-classical trajectory programs. For each molecular system, depending on whether it is diatomic, triatomic, or tetratomic, one, three, or six different bound distances are analyzed and compared with the breaking up or cutting distance. The fragments are then determined accordingly, and the *group* matrix is updated, creating new molecular systems for the fragments, and deleting the information related to the original molecular system.

In the second step, the forming procedure, the program determines which

new collisions (molecular systems) must be considered. This is defined when one of the distances between the atoms of two systems is inferior to the forming distance. For a collision involving up to four atoms, the resulting PES is randomly defined according to the spin, symmetry, and angular momentum probabilities quoted in Tab. 2. It should be noted that in the case of simultaneous collisions involving more than two molecular systems, only two of them are considered in each integration step.

It is considered that reactive collisions occur mainly through the ground and the first excited state PESs that we have implemented. Suppose there is an implemented PES for the selected state. In that case, the *group* matrix is updated, creating a new molecular system and deleting the information referring to the colliding fragments.

Owing to a lack of a PES available for the selected excited state, it is considered a non-reactive collision. To avoid the repetition of the treatment of this collision in subsequent steps, the *group* matrix information is updated, recording the identity of the colliding partners. Similar information is kept for all the collisions involving more than four atoms. These collisions are considered to proceed along a non-reactive potential. This treatment allows energy transfer between the colliding partners but avoids the formation of new bonds.

The way the non-reactive collisions are treated deserves particular attention. The information related to the non-reactive collision will be lost for both partners in the breaking procedure when the distance between them is greater than the breaking distance or if, in the forming procedure, one of the partners initiates a new collision with a third one.

This approach to building a gPES faces two continuity problems. One is related to the breaking and forming distances that should be large enough for the interaction energy between the fragments to be disregarded. A large value for these distances has the drawback of increasing the three-body collision probability. The other derives from inconsistencies in the PESs used to represent the molecular system and the fragments, *i.e.*, the energy and derivatives of the fragments computed using the molecular system PES should be the same as the sum of the values computed with their PESs. This condition is accomplished when using a many-body expansion [7] to build the PESs for large systems, but it hardly happens when using PESs from different authors. Such is the case for some of the implemented potentials. Both problems give rise to discontinuities in the total potential energy, and the difference in the derivatives introduces small discontinuities in the acceleration. To ensure energy conservation below 2 kcal/mol throughout the simulation, N-dimensional switch functions are employed during transitions between PESs[5].

## 2.2 Integration

MReaDy uses the well-known velocity Verlet algorithm to integrate the motion equations for each atom in the mixture in cartesian coordinates. It is represented by Eq. 4,

$$\mathbf{r}_{n+1} = \mathbf{r}_n + \mathbf{v}_n \Delta t + \frac{1}{2} \mathbf{a}_n (\Delta t)^2 \qquad (1)$$

$$\mathbf{v}_{n+\frac{1}{2}} = \mathbf{v}_n + \frac{1}{2} \mathbf{a}_n \Delta t \qquad (2)$$

$$\mathbf{a}_{n+1} = \mathbf{F}(\mathbf{r}_{n+1})/m \qquad (3)$$

$$\mathbf{v}_{n+1} = \mathbf{v}_{n+\frac{1}{2}} + \frac{1}{2} \mathbf{a}_{n+1} \Delta t \qquad (4)$$

In the above equations, $\mathbf{r}_n$, $\mathbf{v}_n$, and $\mathbf{a}_n$ represent the position, velocity, and acceleration at time step $n$ respectively. $\mathbf{F}(\mathbf{r}_{n+1})$ is the force acting on the particle at the updated position $\mathbf{r}_{n+1}$, $m$ is the mass of the particle, and $\Delta t$ is the time step size. The algorithm updates the position and velocity of the particle at each time step.

## 2.3 Boundary conditions

MReaDy program uses Periodic boundary conditions (Fig. 2), so the number density of the systems is conserved. Nevertheless, care has to be taken to avoid boundary effects [6]. A necessary condition is that the volume in which the atoms are set must be big enough not to be influenced by their reflected copies.
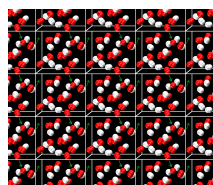


Figure 2: Molecules in a 3D periodic system can enter and leave each cube by crossing through one of its respective six surfaces.

The use of this approximation restricts the scope of the simulations to homogeneous systems. Several other possibilities could be further implemented, like introducing reactive walls or implementing a reactant flux from one of the surfaces.

## 2.4 Input file and setting the initial experimental conditions

Through the input file *parameters.f90* the user sets the experimental conditions and computing parameters for the simulation.

The experimental conditions refer to the kind and initial number of molecular species, temperature and volume (box length). To minimize initial intermolecular potential energy, each system is randomly placed at a position farther than twice the breaking distance from other species previously set. The initial temperature is reflected in the kinetic energy of O and H isolated atoms, $H_2$, $O_2$ and OH molecules. The translational velocity, both for atoms and diatomics, can be randomly generated according to a Maxwell-Boltzmann distribution, using a rejection algorithm, or it can be set to have a constant absolute value corresponding to the average kinetic energy at the chosen temperature, $v = 3k_B T/M_t$. In all cases, MReaDy randomly generates the velocity direction which is defined by the polar and azimuthal angles, $\theta = \arccos(1-2\xi_1)$, and $\phi = 2\pi\xi_2$. Vibrational and rotational motions for the diatoms are also randomly generated

according to the initial temperature taking into account the nuclear spin symmetry of each diatomic when defining the rotational quantum number. The procedure implemented is the one proposed for atom-diatom collisions by Truhlar and Muckerman [31], *i.e.*, after defining the rotational and vibrational quantum numbers from the corresponding partition function, the diatomic is located at the outer turning point. Then, the equations of motion are integrated until a randomly generated fraction of the respective vibrational period is achieved.

To set the computing parameters in the input file (*parameters.f90*), it is necessary to define the breaking distance and forming distance, the time integration step, the total number of steps, the printing step, the backup step, and the seed for the random generator.

Based on backup files, it is possible to restart a calculation at any user's defined step. It allows one to follow specific collisions in detail, if necessary, or to proceed with a calculation in case of a power failure. The integration, printing, backup, and total number of steps can be modified. Re-initialization can be done successively based on the files created in the preceding calculations.

# 3 MReaDy's output

According to the printing step, set by the user, the potential, kinetic, and total energy for the system, the cartesian coordinates, the velocity modulus, and the atom ID for each atom are written to a geo*.xyz file. This file has a format that allows the visualization of molecular motion using the Visual Molecular Dynamics program (VMD) [32].

Whenever a new system is formed or destroyed, it is written to a time_changes*.cvs. This file allows us to study the time evolution of the system.

For re-initialization purposes, two free-format backup files are generated. The first is with the initial conditions, such as the total number of atoms, integration step, and volume. The second file, written according to a user's defined backup step, contains the current step; the *group* matrix giving information regarding the existing systems; the atom species matrix; the cartesian coordinates for all the atoms from the previous and current step; the atoms modulus of the velocity; the potential derivatives; the corresponding atoms mass, and finally, the seed argument for the generation of the random numbers.

The four files mentioned above make up MReaDy's standard output. Moreover, how MReaDy treats information allows a broad range of data output implementation. Such is the case when following the generation and destruction of a specific kind of molecule by printing their positions and velocities. With the data obtained this way, it is possible to develop code to determine information such as the vibrational and rotational states during their existence.

# 4 How to use MReaDy

| | |
|---:|:---|
| Initial conditions : | From the file **units.ods** check initial desired conditions of mixture, pressure and temperature |
| **parameters.f90** : | Where to set initial conditions and parameters such as step and printing time. |
| Compilation : | Executing the **makefile** will create the **mready** executable that can be later renamed. Options such as optimization, parallelization, and debugging are in the file **makefile**. |
| Submitting the process : | Check top or htop commands for 2 free cores (ex. 6 and 7), and submit process. |

```
time taskset -c 6,7 nohup ./MReaDy &
```

| | |
|---:|:---|
| time : | Displays the time taken to complete the process. |
| taskset : | Sets in which cores the process **MReaDy** will run. |
| nohup : | Redirects output from terminal to file **nohup.out**. |
| ./**MReaDy** : | The executable to run. |
| & : | Releases the terminal and leaves the process running in the background. |

# 5 Practical examples

Download Practical.zip package to your Desktop.
Open terminal
Unpack in Desktop with:
tar -zxfv Practical.zip

Although the user can and should define the way folders are arranged, we present a simple example of how to do it. The folder **Practical** has the following items:

| | |
|---:|:---|
| bin : | Where the executable is located, and where we will obtain the output data, especially inside the folder **out**. It is also recommended for a copy of the parameters.f90 be kept here. |
| graphs : | Where graphics should be created. |
| MReaDy : | Where the files for compiling are. |
| plot : | Where files for plotting and other data process is located. |
| units.ods : | File to help determine working physical and chemical conditions. |

Concept of the problem:

- What is the composition
- How many atoms
- At what pressure and temperature
- Check file units.ods

Output files:

- nohup
- geo.xyz

- time_changes.cvs
- Backup files

Check the file **units.ods** to look for the right parameters to set working conditions for the simulations between 10,30,50 atm, and 1500,2000, 2500 K.

Use file **Parameters.f90** to set the values for working conditions such as:

- Number and type of molecules in the system
- Temperature (Boltzman or fixed)
- Printing and backup time

Observe **makefile** and the options for compiling. Compile. Check the availability of cores in the computer and submit the processes.

While MReaDy is running, observe the several files in the program and how it is organized.

- makefile
- mready.f90
- parameters.f90
- read_input_file.f90
- generate*_files.f90
- agrupa.f90
- desagrupa.f90
- potential.f90
- verlet.f90
- write_geom.f90
- generate_*.f90
- PES and PEF files and respective switches for transition to fragments.
- kdtree2_mr.f90

Some recurrent tools can be used with MReaDy, namely:

- VMD - Visual Molecular Dynamics program
- Gnuplot
- ministats

Check **plot** folder and its scripts for bash and Gnuplot

When the program ends, run **./multi.sh** script to obtain graphics.

Try to reinitialize the program in the middle of the steps and make it with a lower printing time.

Make new graphics and use VMD with new data files

Printing information every time a specific event happens, like a molecule breaking is possible. Check **fort.10** for information.

# 6 Some useful tips

## 6.1 Generical commands

|  |  |
|---:|:---|
| grep : | Obtaining all lines with string "Step". |
|  | grep "Step" geo0.xyz |
| head, tail : | Obtain beginning or end of file. |
| Pipping : | Treat results from a first to a second command. |
|  | `grep "Step" geo0.xyz | [head,tail,sort,awk, etc]` |
| Saving to new file : | grep "Step" geo0.xyz > geo0.dat |
| From awk : | `awk '{print $2, $9}' geo0.dat | \` |
|  | `gnuplot -p -e 'plot "-" u ($1*0.05E-15):2 t "Pot E"'` |

## 6.2 Graphics in Terminal with Gnuplot

|  |  |
|---:|:---|
| From file : | `gnuplot -p -e 'plot "geo0.dat" u ($2*0.05E-15):9'` |
| Pipping : | `cat geo0.dat | \` |
|  | `gnuplot -p -e 'plot "-" u ($2*0.05E-15):9 t "Pot E"'` |
| From awk : | `awk '{print $2, $9}' geo0.dat | \` |
|  | `gnuplot -p -e 'plot "-" u ($1*0.05E-15):2 t "Pot E"'` |

## 6.3 Statistics

|  |  |
|---:|:---|
| ministats : | The ministats command calculates fundamental statistical properties of numeric data in the specified files or, if no file is specified, standard input. |
|  | ministats -C 9 geo0.dat |

# Index

# References

[1] C. Mogo, J. Brandão, The MReaDy program: Building a global potential energy surface and reactive dynamic simulations for the hydrogen combustion, Journal of Computational Chemistry 35 (17) (2014) 1330–1337. doi:10.1002/jcc.23621.

[2] D. V. Coelho, J. Brandão, C. Mogo, Internal energy and temperature of a carbon nanotube, Fullerenes, Nanotubes and Carbon Nanostructures 0 (0) (2022) 1–5. doi:10.1080/1536383X.2022.2031164.

[3] C. Mogo, J. Brandão, W. Wang, D. Coelho, C. Rio, Quasiclassical study of a termolecular reaction: Application to the $HO_2$ collisional stabilization process, Computational and Theoretical Chemistry 1209 (2022) 113614. doi:https://doi.org/10.1016/j.comptc.2022.113614.

[4] Mogo, C., Brandão, J., Wang, W., Coelho, D. & Rio, C. Quasiclassical study of a termolecular reaction: A more detailed description of the HO2 collisional stabilization process. *Computational And Theoretical Chemistry.* **1224** pp. 114123 (2023), https://www.sciencedirect.com/science/article/pii/S2210271X23001056

[5] C. Mogo, J. Brandão, N-dimensional switch function for energy conservation in multiprocess reaction dynamics, Journal of Computational Chemistry 37 (16) (2016) 1521–1524. doi:10.1002/jcc.24361.

[6] A. M. P., T. D. J., Computer Simulation of Liquids, Oxford University Press, 2000.

[7] J. N. Murrell, S. Carter, S. C. Farantos, P. Huxley, A. J. C. Varandas, Molecular Potential Energy Functions, Wiley, Chichester, 1984.

[8] M. Jacobson, W. Colella, D. Golden, Cleaning the air and improving health with hydrogen fuel-cell vehicles, Science 308 (5730) (2005) 1901–1905.

[9] S. P. Walch, Extended active space CASSCF/MRSD CI calculations of the barrier height for the reaction $O+H_2 \rightarrow OH+H$, The Journal of Chemical Physics 86 (10) (1987) 5670–5675.

[10] J. Hua, M. Wu, K. Kumar,Numerical simulation of the combustion of hydrogen–air mixture in micro-scaled chambers. Part I: Fundamental study, Chemical Engineering Science 60 (13) (2005) 3497–3506.

[11] M. Ó Conaire, H. J. Curran, J. M. Simmie, W. J. Pitz, C. K. Westbrook, A comprehensive modelling study of hydrogen oxidation, International Journal of Chemical Kinetics 36 (11) (2004) 603–622.

[12] P. Saxena, F. A. Williams, Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide, Combustion and Flame 145 (1–2) (2006) 316 – 323.

[13] P. Boivin, A. L. Sánchez, F. A. Williams, Explicit analytic prediction for hydrogen–oxygen ignition times at temperatures below crossover, Combustion and Flame 159 (2) (2012) 748 – 752.

[14] F. L. Dryer, M. Chaos, Ignition of syngas/air and hydrogen/air mixtures at low temperatures and high pressures: Experimental data interpretation and kinetic modeling implications, Combustion and Flame 152 (1–2) (2008) 293 – 299.

[15] S. P. Medvedev, G. L. Agafonov, S. V. Khomik, B. E. Gelfand, Ignition delay in hydrogen–air and syngas–air mixtures: Experimental

data interpretation via flame propagation, Combustion and Flame 157 (7) (2010) 1436 – 1438.

[16] T. W. Rosch, E. J. Maginn, Reaction ensemble monte carlo simulation of complex molecular systems, Journal of Chemical Theory and Computation 7 (2) (2011) 269–279.

[17] C. Heath Turner, J. K. Brennan, M. Lísal, , W. R. Smith, J. Karl Johnson, K. E. Gubbins, Simulation of chemical reaction equilibria by the reaction ensemble monte carlo method: a review†, Molecular Simulation 34 (2) (2008) 119–146.

[18] A. C. Van Duin, S. Dasgupta, F. Lorant, W. A. Goddard, Reaxff: a reactive force field for hydrocarbons, The Journal of Physical Chemistry A 105 (41) (2001) 9396–9409.

[19] A. I. Boothroyd, W. J. Keogh, P. G. Martin, M. R. Peterson, A refined h potential energy surface, The Journal of chemical physics 104 (1996) 7139.

[20] A. I. Boothroyd, P. G. Martin, W. J. Keogh, M. J. Peterson, An accurate analytic H_4 potential energy surface, The Journal of Chemical Physics 116 (2) (2002) 666–689.

[21] J. Brandão, C. M. A. Rio, Double-valued potential energy surface for H_2O derived from accurate ab initio data and including long-range interactions, The Journal of Chemical Physics 119 (6) (2003) 3148–3159.

[22] G. sheng Wu, G. C. Schatz, G. Lendvay, D.-C. Fang, L. B. Harding, A new potential surface and quasiclassical trajectory study of H + H_2O → OH + H_2, The Journal of Chemical Physics 113 (8) (2000) 3150–3161.

[23] J. Brandão, C. Mogo, B. C. Silva, Potential energy surface for H_2O($^3$A") from accurate ab initio data with inclusion of long-range interactions, The Journal of Chemical Physics 121 (18) (2004) 8861–8868.

[24] C. M. A. Rio, J. Brandão, A potential energy surface for ground triplet state of H_2O_2 (2013) to be published.

[25] J. Brandão, C. M. A. Rio, J. Tennyson, A modified potential for ho[sub 2] with spectroscopic accuracy, The Journal of Chemical Physics 130 (13) (2009) 134309.

[26] D. Coelho, J. Brandão, A potential energy surface for ground singlet state of H_2O_2 (2013) to be published.

[27] A. J. C. Varandas, A. A. C. C. Pais, J. M. C. Marques, W. Wang, On the chaperon mechanism for association rate constants: the formation of ho2 and o3, Chemical Physics Letters 249 (3–4) (1996) 264 – 271.

[28] A. J. C. Varandas, H. G. YU, Double many-body expansion potential energy surface for ground-state HO_3, Molecular Physics 91 (2) (1997) 301–318.

[29] A. J. C. Varandas, W. Wang, On the o2($\nu$') + o2($\nu$') atmospheric reaction: a quasiclassical trajectory study, Chemical Physics 215 (2) (1997) 167 – 182.

[30] A. J. C. Varandas, Energy switching approach to potential surfaces. an accurate single-valued function for the water molecule, J. Chem. Phys. 105 (9) (1996) 3524–3531.

[31] D. G. Truhlar, J. T. Muckerman, Reactive scattering cross sections iii. quasiclassical and semiclassical methods, in: R. B. Bernstein (Ed.), Atom-Molecule Collision Theory, 2nd Edition, Plenum Press, New York, 1984, pp. 505–566.

[32] W. Humphrey, A. Dalke, K. Schulten, VMD – Visual Molecular Dynamics, Journal of Molecular Graphics 14 (1996) 33–38.

[33] J. C. Ianni, A comparison of the bader-deuflhard and the cash-karp runge-kutta integrators for the gri-mech 3.0 model based on the chemical kinetics code kintecus, Computational Fluid and Solid Mechanics (2003) 1368–1372.