Online Supplement for
Surrogate optimization of computationally expensive black-box problems with hidden constraints

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1 Details of the Individual Algorithm Steps

In the following, we show a more detailed step-by-step description of the algorithm that is described in Section 3 in the main document. We recommend that the reader reads the main document (Sections 3.1-3.3) alongside the below algorithm steps.

Algorithm 1 SHEBO Surrogate model algorithm for hidden constraints

1: Input parameters: $n_{\max}$ (maximum number of allowed evaluations), n_0 (size of initial experimental design), n_{mads} (number of evaluations done by MADS), $\mathcal{W}$ (weight pattern) (see Table 2 in the main paper for default values).
2: Create an initial experimental design with n_0 points by Latin hypercube sampling. Denote the set of points by $\mathcal{S}$.
3: Do the expensive function evaluations and collect the function values in the set $\mathcal{Y}$ (NaN for failed evaluations).
4: Divide the points in $\mathcal{S}$ into successfully evaluated points $\mathcal{S}_e$ and failed points $\mathcal{S}_u$, i.e. $\mathcal{S} = \mathcal{S}_e \cup \mathcal{S}_u$.
5: Compute rank($\mathbf{P}_e$), where $\mathbf{P}_e$ is the sample site matrix augmented with a column vector of ones (see equation (4) in the main document). Keep adding points to $\mathcal{S}$ until the rank condition for $\mathbf{P}_e$ is satisfied.
6: Set $n = |\mathcal{S}|$. Set $i = 1$.
7: Find the best function value (denote $f_{\min}$) and the corresponding sample point $\mathbf{x}_{\min}$.
8: Sample stage = local search.
9: **while** $n < n_{\max}$ **do**
10:     Select the new sample point $\mathbf{x}_{\text{new}}$ as follows:
11:     **if** Sample stage = local search **then**
12:         Compute the surrogate model parameters for s_e and s_g based on the current sampling history.
13:         Solve an auxiliary optimization problem that finds the minimum of the surrogate model of the objective function s_e subject to the evaluability constraint defined in equation (6b) in the main document. $\mathbf{x}_{\text{new}}$ is the solution of the auxiliary problem.
14:         Sample stage = transition search(i).
15:     **else if** Sample stage = transition search(i) **then**
16:         Add random perturbations to $\mathbf{x}_{\min}$ and use scoring method to select $\mathbf{x}_{\text{new}}$ (see Algorithm 2 in the main document and Section 2 below for more details).
17:         **if** $i < |\mathcal{W}|$ **then**
18:             Update $i \leftarrow i + 1$.
19:         **else**
20:             Sample stage = Global search.
21:             Set $i = 1$.
22:         **end if**

else
Global search: Select $\mathbf{x}_{\text{new}}$ as a point that maximizes the minimum distance to $\mathcal{S}$.
Sample stage = local search.
end if
Do the expensive evaluation at $\mathbf{x}_{\text{new}}$, $f_{\text{new}} = f(\mathbf{x}_{\text{new}})$.
Update $\mathcal{S} = \mathcal{S} \cup \{\mathbf{x}_{\text{new}}\}$, $\mathcal{Y} = \mathcal{Y} \cup \{f_{\text{new}}\}$, $n = n + 1$.
if $f_{\text{new}} < f_{\min}$ **then**
$f_{\min} = f_{\text{new}}$; $\mathbf{x}_{\min} = \mathbf{x}_{\text{new}}$.
Do a local search with MADS for at most n_{mads} evaluations starting at $\mathbf{x}_{\min}$ and denote the sample points and function values by $\mathcal{X}$ and $\mathcal{Y}_{\mathcal{X}}$, respectively.
Update $\mathcal{S} = \mathcal{S} \cup \mathcal{X}$, $\mathcal{Y} = \mathcal{Y} \cup \mathcal{Y}_{\mathcal{X}}$, $n = n + |\mathcal{X}|$.
Update $f_{\min}$ and $\mathbf{x}_{\min}$ if necessary.
end if
end while
return $\mathbf{x}_{\min}$, $f_{\min}$.

2 Scoring Method in Transition Search

In order to score the candidate points in the transition search, we closely follow Regis and Shoemaker (2007). For each candidate point $\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_{n_{\text{cand}}}$, we compute the distance to the set $\mathcal{S}$:

$$\Delta_j = \min_{\mathbf{x}_l \in \mathcal{S}} \|\mathbf{x}_l - \boldsymbol{\xi}_j\|_2, \; j = 1, \ldots, n_{\text{cand}}.$$

We scale the distance values to [0,1] according to

$$V_D(\boldsymbol{\xi}_j) = \frac{\Delta_{\max} - \Delta_j}{\Delta_{\max} - \Delta_{\min}},$$

where $\Delta_{\max} = \max\{\Delta_j, j = 1, \ldots, n_{\text{cand}}\}$ and $\Delta_{\min} = \min\{\Delta_j, j = 1, \ldots, n_{\text{cand}}\}$.

We use the radial basis function surrogate model of the objective function to predict the function values for $\boldsymbol{\xi}_j, \; j = 1, \ldots, n_{\text{cand}}$, denoted by $s_e(\boldsymbol{\xi}_j), \; j = 1, \ldots, n_{\text{cand}}$. We scale these values to [0,1] according to

$$V_R(\boldsymbol{\xi}_j) = \frac{s_e(\boldsymbol{\xi}_j) - s_e^{\min}}{s_e^{\max} - s_e^{\min}},$$

where $s_e^{\max} = \max\{s_e(\boldsymbol{\xi}_j), \; j = 1, \ldots, n_{\text{cand}}\}$ and $s_e^{\min} = \min\{s_e(\boldsymbol{\xi}_j), \; j = 1, \ldots, n_{\text{cand}}\}$.

We combine both scores in a weighted sum:

$$V(\boldsymbol{\xi}_j) = w_s V_R(\boldsymbol{\xi}_j) + (1 - w_s) V_D(\boldsymbol{\xi}_j), \; j = 1, \ldots, n_{\text{cand}},$$

where w_s is chosen from the weight pattern $\mathcal{W}$ (see Table 2 in the main document), and the candidate point with the lowest score is chosen as the new sample point.

3 Numerical test problems

In the following, we provide the analytic descriptions of the test problems that we used. Sections 3.1-3.11 discuss the analytic test problems that have variable dimension d, $d \in \{2, 5, 10, 20, 30\}$. Section 3.12 offers more details of the combustion application. For the analytic test problems, 3.1-3.11, we use constraint functions $c(\mathbf{x}) \leq 0$ for defining the regions in which the objective function is evaluable. If a point $\mathbf{x}$ satisfies the constraint, it means a function value can be computed. If the point does not satisfy the constraint, no function value can be obtained and the objective function value is NaN. In the numerical experiments, we treat the constraints and objective functions as black-boxes, i.e., the algorithms are not able to take advantage of the analytical descriptions. We use this approach in order to investigate the algorithm's performance for problems with different characteristics, such as simply connected and disconnected evaluability regions. Using fast-to-evaluate analytical test problems speeds up the numerical experiments and gives us a sense of the efficiency and scalability of the algorithms for larger dimensions. We derived the problem formulations by combining widely-used benchmark problems which can be found here `http://infinity77.net/global_optimization/genindex.html` (last accessed April 2, 2018). The combination of objective and constraint functions has been chosen by the authors.

3.1 Test problem 1

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ -20\exp\left(-0.2\sqrt{\frac{1}{d}\sum_{i=1}^{d} x_i^2}\right) - & \\ \quad \exp\left(\frac{1}{d}\sum_{i=1}^{d}\cos(2\pi x_i)\right) + 20 + \exp(1) & \text{else} \end{cases} \tag{1a}$$

$$x_i \in [-10, 10], i = 1, \dots, d \tag{1b}$$

$$c(\mathbf{x}) = \begin{cases} 1 & \text{if } \quad -0.2 \le x_i \le 0.2 \ \forall i = 1, \dots, d \\ \sum_{i=1}^{d} x_i \sin(x_i) + 0.1 x_i & \text{else} \end{cases} \tag{1c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective function is the Ackley function and the constraint is a variant of the Alpine01 function.

3.2 Test problem 2

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ (x_1 - x_2)^2 + \exp\left((1 - \sin(x_1))^2\right)\cos(x_2) + & \\ \quad \exp\left((1 - \cos(x_2))^2\right)\sin(x_1) & \text{else} \end{cases} \tag{2a}$$

$$x_i \in [-3\pi, 3\pi], i = 1, \dots, d \tag{2b}$$

$$c(\mathbf{x}) = \sum_{i=1}^{d} \Bigg[x_i \sin\left(\sqrt{|x_1 - x_i + 1|}\right)\cos\left(\sqrt{|x_1 + x_i + 1|}\right) + (x_1 + 1)\sin\left(\sqrt{|x_1 + x_i + 1|}\right)\cos\left(\sqrt{|x_1 - x_i + 1|}\right)\Bigg] - 5 \tag{2c}$$

This problem has one connected region with evaluable points and with several local minima. The objective function is the Bird function and the constraint is derived from the Rana function.

3.3 Test problem 3

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ -\left(\sum_{i=1}^{d} x_i^2 + 25\sum_{i=1}^{d}\sin^2(x_i)\right) & \text{else} \end{cases} \tag{3a}$$

$$x_i \in [0, 10], i = 1, \dots, d \tag{3b}$$

$$c(\mathbf{x}) = \sum_{i=1}^{d} \left[\sin^2\left(1 - \frac{16}{15}x_i\right) - \frac{1}{50}\sin\left(4 - \frac{64}{15}x_i\right) - \sin\left(1 - \frac{16}{15}x_i\right)\right] - 1 \tag{3c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective function is derived from the Eggcrate function and the constraint is derived from the Giunta function.

3.4 Test problem 4

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ \left[\sum_{i=0}^{4}(i+1)\cos(ix_1+i+1)\right] \times & \\ \qquad \left[\sum_{i=0}^{4}(i+1)\cos\left((i+2)x_2+i+1\right)\right] - 0.1 & \text{else} \end{cases} \tag{4a}$$

$$x_i \in [0, 10], i = 1, \ldots, d \tag{4b}$$

$$c(\mathbf{x}) = \prod_{i=1}^{d} [\sqrt{x_i}\sin(x_i)] + 1 \tag{4c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is derived from the Hansen function. The constraint is derived from the Alpine02 function.

3.5 Test problem 5

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ 10d\sum_{i=1}^{d}\left[x_i^2 - 10\cos(2\pi x_i)\right] & \text{else} \end{cases} \tag{5a}$$

$$x_i \in [-5, 5], i = 1, \ldots, d \tag{5b}$$

$$c(\mathbf{x}) = -\left(\sin^2(\pi y_1) + \sum_{i=1}^{d-1}(y_i-1)^2\left(1+10(\sin^2(\pi y_{i+1}))\right) + (y_d-1)^2 - 4d\right) \tag{5c}$$

$$y_i = 1 + \frac{x_i - 1}{4}, i = 1, \ldots, d \tag{5d}$$

This problem has several disconnected regions with evaluable points. The objective is the Rastrigin function. The constraint is derived from the Levy03 function.

3.6 Test problem 6

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ -20\exp\left(-0.2\sqrt{\frac{1}{d}\sum_{i=1}^{d}x_i^2}\right) - & \\ \qquad \exp\left(\frac{1}{d}\sum_{i=1}^{d}\cos(2\pi x_i)\right) + 20 + \exp(1) & \text{else} \end{cases} \tag{6a}$$

$$x_i \in [-5, 5], i = 1, \ldots, d \tag{6b}$$

$$c(\mathbf{x}) = -\left(\sin^2(\pi y_1) + \sum_{i=1}^{d-1}(y_i-1)^2(1+10(\sin^2(\pi y_{i+1}))) + (y_d-1)^2 - 4d\right) \tag{6c}$$

$$y_i = 1 + \frac{x_i - 1}{4}, i = 1, \ldots, d \tag{6d}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is the Ackley function and the constraint is derived from the Levy03 function.

3.7 Test problem 7

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ \sum_{i=1}^{d} \left[x_i \sin(x_i) + 0.1 x_i \right] & \text{else} \end{cases} \tag{7a}$$

$$x_i \in [-12, 12], i = 1, \ldots, d \tag{7b}$$

$$c(\mathbf{x}) = -\sum_{i=1}^{d} \left[x_i \sin(\sqrt{|x_i|}) \right] + 2 \tag{7c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is derived from the Alpine01 function and the constraint is derived from the Schwefel26 function.

3.8 Test problem 8

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ \sum_{i=1}^{d} \sum_{j=1}^{5} \left[j \sin((j+1)x_i) + j \right] & \text{else} \end{cases} \tag{8a}$$

$$x_i \in [-10, 10], i = 1, \ldots, d \tag{8b}$$

$$c(\mathbf{x}) = \sum_{i=1}^{d} \left[x_i^4 - 16 x_i^2 + 5 x_i \right] - 10d \tag{8c}$$

This problem has one connected region with evaluable points and with several local minima. The objective is the Shubert03 test function and the constraint is derived from the Styblinski-Tang function.

3.9 Test problem 9

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ 1 - \frac{1}{d} \sum_{i=1}^{d} \left[\cos(10 x_i) \exp(-x_i^2/2) \right] & \text{else} \end{cases} \tag{9a}$$

$$x_i \in [-\pi, \pi], i = 1, \ldots, d \tag{9b}$$

$$c(\mathbf{x}) = -\left(\sum_{i=1}^{d} |x_i \sin(x_i) + 0.1 x_i| - d \right) \tag{9c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is the Wavy test function and the constraint is derived from the Alpine01 function.

3.10 Test problem 10

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ -20 \exp\left(-0.2 \sqrt{\frac{1}{d} \sum_{i=1}^{d} x_i^2} \right) - & \\ \quad \exp\left(\frac{1}{d} \sum_{i=1}^{d} \cos(2\pi x_i) \right) + 20 + \exp(1) & \text{else} \end{cases} \tag{10a}$$

$$x_i \in [0.25, 10], i = 1, \ldots, d \tag{10b}$$

$$c(\mathbf{x}) = -\sum_{i=1}^{d} \sin(10 \log(x_i)) \tag{10c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is the Ackley function and the constraint is derived from the Vincent function.

3.11 Test problem 11

$$\min_{\mathbf{x}} f(\mathbf{x}) = \begin{cases} NaN & \text{if } c(\mathbf{x}) > 0 \\ \sum_{j=1}^{d} \left\{ \sum_{i=1}^{20} \left[0.5^i \cos(2\pi 3^i (x_j + 0.5)) \right] \right. & \\ \quad \left. -d \sum_{i=1}^{20} \left[0.5^i \cos(\pi 3^i) \right] \right\} & \text{else} \end{cases} \tag{11a}$$

$$x_i \in [0.25, \pi], i = 1, \ldots, d \tag{11b}$$

$$c(\mathbf{x}) = -\sum_{i=1}^{d} \sin(10 \log(x_i)) \tag{11c}$$

This problem has several disconnected regions with evaluable points and with several local minima. The objective is the Weierstrass function and the constraint is derived from the Vincent function.

3.12 Combustion Application Problem

The combustion model $\mathcal{M}(\mathbf{x})$ depends on a vector of d "active" parameters[1], $\mathbf{x}$, and produces $\mathbf{z}$, an approximation to a vector of n_z measurable outputs. The kinetics component of this model is specified in ChemKin-II (Kee et al. 1989) format. The Arrhenius form of the model requires that $\mathbf{x}$ be constrained in various ways, for example, to avoid negative equilibrium constants. If the measurement uncertainty is denoted by $\mathbf{v}$, then $\mathbf{z} = \mathcal{M}(\mathbf{x}) + \mathbf{v}$. Given an uncertain distribution of $\mathbf{x}$, we can estimate the likelihood that $\mathbf{z}$ will match experimentally measured data. Using Bayes' rule

$$p(\mathbf{x}|\mathbf{z}) = p_{\mathbf{x}}(\mathbf{x})\, p(\mathbf{z}|\mathbf{x})$$

where $p_{\mathbf{x}}(\mathbf{x})$ is the probability distribution of parameters and $p(\mathbf{z}|\mathbf{x})$ is the resulting distribution of predicted data. Assume $p_{\mathbf{x}}(\mathbf{x})$ and $\mathbf{v}$ are Gaussian. If $\mathcal{M}$ is linear, then $p(\mathbf{x}|\mathbf{z})$ is also Gaussian, and so its posterior would be completely determined by its mean and variance. The mean can be found by minimizing the quantity

$$F(\mathbf{x}) = -\log p(\mathbf{x}|\mathbf{z}) = -\log p_{\mathbf{x}}(\mathbf{x}) - \log p(\mathbf{z}|\mathbf{x}) + C$$

up to some constant, C. Define the minimizer, $\boldsymbol{\mu} \in \arg\min_{\mathbf{x}} F(\mathbf{x})$. Note that in our case, $\mathcal{M}$ is nonlinear, so $\boldsymbol{\mu}$ becomes the *posterior mode*, and there is no guarantee that there is only a single global posterior mode.

Our problem has $d = 31$ active parameters associated specifically with important combustion intermediate species HO_2 and H_2O_2. Table 1 shows the complete syngas kinetic model parameter set; the active parameters for this study are boxed in the table (**bold** parameters are varied synchronously). The remaining parameters are held fixed throughout this study. We have assembled $n_z = 92$ simulated experiments, consisting of 78 steady unstrained premixed flames at various pressures and mixtures, 6 constant-pressure flow reactors and 8 ignition-delay experiments (72 of the premixed flame cases were taken from Burke et al. (2012) and references therein; the remaining were taken from Davis et al. (2005)). The premixed flame cases were simulated using PREMIX (Kee et al. 1998); for each, the relevant data extracted was the propagation speed of the steady, unstrained flame. The flow reactor and ignition delay experiments were simulated as point (zero-D) reactors in constant pressure and volume, respectively, using the backward-difference integration method in VODE (Brown et al. 1989); the data extracted from each of these simulations is detailed in the relevant references, as are the measured values and experimental errors of all experiments used.

[1] "Active parameters" refers to the subset of parameters that we are optimizing. There are more parameters than the ones reported below, but for these other parameters we use the default values given by Davis et al. (2005).

Table 1: Arrhenius rate parameters for syngas combustion model (kinetics, and accompanying thermodynamics and transport – in Kee et al. (1989) format). Parameter database taken from Burke et al. (2012), except for the final two, which were taken from Davis et al. (2005). For this study, the 32 boxed parameters are "active" (i.e., subject to optimization); all others are considered fixed. The two **bold** parameters are varied synchronously; giving 31 independent parameters. The forward rate constant, $K_f = AT^{\beta}\exp\left(-E_a/RT\right)$. *The number in parentheses is the exponent of 10, i.e., 2.65(16) = 2.65 × 10^{16}. For the active parameters lower and upper bounds are provided in the last column.

RID	Reaction			A*	β	E_a	Bounds L:U
1	H + O_2	=	O + OH	1.04(14)	0	15286	
2	O + H_2	=	H + OH	3.818(12)	0	7948	
3	O + H_2	=	H + OH	8.792(14)	0	19170	
4	OH + H_2	=	H + H_2O	2.16(8)	1.51	3430	
5	2 OH	=	O + H_2O	3.34(4)	2.42	-1930	
6	H_2 + M	=	2 H + M	4.577(19)	-1.40	104380	
	Third-body: H_2(2.5), H_2O(12), Ar(0), He(0)						
7	H_2 + Ar	=	2 H + Ar	5.84(18)	-1.10	104380	
8	H_2 + He	=	2 H + He	5.84(18)	-1.10	104380	
9	2 O + M	=	O_2 + M	6.165(15)	-0.5	0	
	Third-body: H_2(2.5), H_2O(12), Ar(0), He(0)						
10	2 O + Ar	=	O_2 + Ar	1.886(13)	0	-1788	
11	2 O + He	=	O_2 + He	1.886(13)	0	-1788	
12	O + H + M	=	OH + M	4.714(18)	-1	0	
	Third-body: H_2(2.5), H_2O(12), Ar(0.75), He(0.75)						
13	H_2O + M	=	H + OH + M	6.064(27)	-3.322	120790	
	Third-body: H_2(3), H_2O(0), He(1.1), N_2(2), O_2(1.5)						
14	2 H_2O	=	H + OH + H_2O	1.006(26)	-2.44	120180	
15	H + O_2 (+M)	=	HO_2 (+M)				
	high pressure, $K_{f\infty}$			$\boxed{4.65084(12)}$	0.44	0	2(12):1(13)
	low pressure, K_{f0}			$\boxed{6.366(20)}$	-1.72	524.8	0:8(20)
	TROE: $F_c = 0.5$						
	Third-body:			H_2($\boxed{2.0}$)			0:6
				H_2O($\boxed{14}$)			0:28
				O_2($\boxed{0.78}$)			0:3
				Ar($\boxed{0.67}$)			0:3
				He($\boxed{0.8}$)			0:3
16	HO_2 + H	=	H_2 + O_2	$\boxed{2.750(6)}$	2.09	-1451	1(6):5(16)
17	HO_2 + H	=	2 OH	$\boxed{7.079(13)}$	0	295	2(13):1(14)
18	HO_2 + O	=	OH + O_2	$\boxed{2.850(10)}$	1	-723.93	1(9):1(11)
19	HO_2 + OH	=	O_2 + H_2O	$\boxed{2.890(13)}$	0	-497	1(13):6(13)
20	2 HO_2	=	O_2 + H_2O_2	$\boxed{4.200(14)}$	0	11982	1(14):2(15)
21	2 HO_2	=	O_2 + H_2O_2	$\boxed{1.300(11)}$	0	-1630	5(10):4(11)
22	H_2O_2 (+M)	=	2 OH (+M)				
	high pressure, $K_{f\infty}$			$\boxed{2.00(12)}$	0.9	48749	5(11):1(12)
	low pressure, K_{f0}			$\boxed{2.49(24)}$	-2.3	48749	1(23):1(25)
	TROE: $F_c = 0.43$						
	Third-body:			H_2($\boxed{3.7}$)			0:15
				H_2O($\boxed{7.5}$)			0:20
				H_2O_2($\boxed{7.7}$)			0:20
				O_2($\boxed{1.2}$)			0:5
				N_2($\boxed{1.5}$)			0:5
				He($\boxed{0.65}$)			0:4
23	H_2O_2 + H	=	OH + H_2O	$\boxed{2.410(13)}$	0	3970	5(11):1(14)
24	H_2O_2 + H	=	HO_2 + H_2	$\boxed{4.820(13)}$	0	7950	1(12):9(13)
25	H_2O_2 + O	=	OH + HO_2	$\boxed{9.550(6)}$	2	3970	1(5):3(7)
26	H_2O_2 + OH	=	HO_2 + H_2O	$\boxed{1.740(12)}$	0	318	5(10:5(12)
27	H_2O_2 + OH	=	HO_2 + H_2O	$\boxed{7.590(13)}$	0	7270	4(12):4(14)
28	HO_2 + H	=	H_2O + O	$\boxed{3.97(12)}$	0	671	1(12):9(12)
29	O + OH + M	=	HO_2 + M	$\boxed{8.000(15)}$	0	0	2(15):2(16)
	Third-body:			H_2($\boxed{2}$)			0:6
				H_2O($\boxed{12}$)			0:35
				Ar($\boxed{\mathbf{0.7}}$)			0:3
				He($\boxed{\mathbf{0.7}}$)			0:3

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