Table S1 Database

Type	Scale	Source and description
DEM	90 m	Resources and Environment Science Data Centre, CAS（https://www.resdc.cn/Default.aspx）
Soil	1:1000000	National Cryosphere Desert Data Centre (www.ncdc.ac.cn) Harmonized World Soil Database (HWSD version 1.1) Some soil attribute parameters are calculated by SPAW (a soil water characteristic model developed by Washington State University)
Land use	1 km	Resources and Environment Science Data Centre, CAS（https://www.resdc.cn/Default.aspx） It is based on Landsat TM image of American Landsat satellite; it is generated by artificial visual interpretation. The land use types include 6 first-class types and 25 second-class types, including woodland, grassland, water, cultivated land, construction land and unused land.
Meteorological data	Daily	China Meteorological Data Service Centre（http://data.cma.cn） Daily data of China's surface climate from 2000 to 2019 (V3.0) and from 149 meteorological stations, mainly including 8 types of data: PRS, TEM, RHU, PRE, EVP, WIN, GST.
Hydrological data	Monthly	Monthly flow of 6 hydrological stations in 2009-2019 (Tangnaihai, Lanzhou,Shizuishan, Toudaoguai, Sanmenxia)

Table S2 Parameters of four large reservoirs in Yellow River basin

Name and Unit	Parameters	Longyangxia	Liujiaxia	Wanjiazhai	Xiaolangdi
Number	OID	1	2	3	5
Sub-basin	SUBBASIN	47	29	11	39
Starting operation time of reservoir (month)	MORES	0	0	0	0
Starting operation time of reservoir (years)	IYRES	0	0	0	0
Water surface area (during emergency flood discharge) (ha)	RES_ESA	38000	13000	2811	27200
Storage capacity (during emergency flood discharge) (10^4m^3)	RES_EVOL	2470000	570000	89600	1265000
Water surface area (during normal flood discharge) (ha)	RES_PSA	33500	10500	2500	24200
Storage capacity (during normal flood discharge) (10^4m^3)	RES_PVOL	2170000	450000	80000	1160000
Initial water quantity of reservoir (water quantity at the beginning of simulation) (10^4m^3)	RES_VOL	1994000	298500	33900	782800
Average daily outflow from the spillway (m^3/s)	RES_RR	479.3333	599.1111	393.7778	702.0000

Table S3 Average monthly water use by area

Area	QH	GS	NX	NMG	SX	SHX	HN	description
WURCH1	101.57	116.12	0.00	118.83	743.01	370.65	518.61	Surface water intake Average daily water quantity taken from rivers in this month.（10^4m^3/day）
WURCH2	137.26	125.08	8.96	107.57	506.18	913.78	1038.09	
WURCH3	157.38	702.54	66.39	88.67	833.55	1586.40	2226.65	
WURCH4	212.20	888.42	971.80	1485.50	1008.60	1058.95	1539.90	
WURCH5	350.15	1533.78	1936.52	3761.61	1029.33	251.33	1644.44	
WURCH6	441.60	1530.88	2935.03	2284.47	1173.39	1621.99	2213.88	
WURCH7	492.71	1310.33	2520.75	3109.17	858.58	1704.96	1957.60	

WURCH8	378.89	997.91	2086.06	1342.63	643.99	1164.04	1511.87	
WURCH9	224.39	624.68	133.15	617.53	548.06	300.71	942.18	
WURCH10	192.80	764.34	112.68	4326.69	473.15	74.07	807.98	
WURCH11	257.89	1098.34	1699.33	1473.35	863.00	595.66	650.20	
WURCH12	153.90	105.74	8.09	64.09	896.96	341.12	590.88	
WUSHAL1	18.52	14.14	0.00	40.92	406.69	253.06	177.30	Groundwater intake Average daily water quantity taken from shallow aquifer in this month（10^4m^3/day）
WUSHAL2	24.58	15.20	0.87	37.61	270.74	640.57	355.29	
WUSHAL3	28.01	84.83	6.44	32.78	442.76	1112.95	761.74	
WUSHAL4	37.38	107.61	100.06	525.70	542.37	744.01	526.41	
WUSHAL5	63.27	185.92	196.85	1342.67	565.93	178.93	558.65	
WUSHAL6	79.75	185.76	299.66	780.67	642.42	1137.33	754.88	
WUSHAL7	87.92	158.86	259.06	1116.42	470.75	1200.29	671.72	
WUSHAL8	69.84	120.96	215.07	475.42	344.70	814.50	514.02	
WUSHAL9	42.02	76.07	14.26	216.54	288.27	219.71	319.54	
WUSHAL10	34.92	92.82	12.77	1550.17	260.39	53.55	274.96	
WUSHAL11	48.38	131.25	174.54	526.76	464.45	420.88	215.79	
WUSHAL12	28.50	12.73	0.78	22.47	494.88	250.63	195.75	

Table S4 Parameters for calibration

Parameters	Description	Value	Range
CN2	SCS runoff curve number	Multiply by	-0.5-0.5
SOL_AWC	Effective soil water storage capacity	Multiply by	-0.5-0.5
SOL_K	Saturated hydraulic conductivity of soil	Replace value	-0.5-0.5
ESCO	Soil evaporation compensation factor	Replace value	0-1
GWQMN	Threshold value of shallow aquifer water level	Replace value	0-5000
REVAPMN	Shallow groundwater seepage threshold	Replace value	0-500
CH_K2	Effective hydraulic conductivity coefficient of alluvial layer in main channel	Replace value	-0.01-500
ALPHA_BF	α coefficient of base flow	Replace value	0-1
GW_DELAY	Time delay of groundwater /d	Replace value	0-500
HRU_SLP	Average grade	Replace value	0-1

Table S5 Decision variables

Area	Qinghai	Gansu	Ningxia	Neimenggu	Shanxi	Shannxi	Henan	Shandong
Qinghai	\	\	\	\	\	\	\	\
Gansu	$X1(TWRA_{QHtoGS})$ $X2(TWRI_{QHtoGS})$	\	\	\	\	\	\	\
Ningxia	$X3(TWRA_{QHtoNX})$ $X4(TWRI_{QHtoNX})$	……	\	\	\	\	\	\
Neimenggu	$X5(TWRA_{QHtoNMG})$ $X6(TWRI_{QHtoNMG})$	……	……	\	\	\	\	\
Shanxi	$X7(TWRA_{QHtoSX})$ $X8(TWRI_{QHtoSX})$	……	……	……	\	\	\	\

Shannxi	$X9(TWRA_{QHtoSHX})$ $X10(TWRI_{QHtoSHX})$	……	……	……	……	\	\	\
Henan	$X11(TWRA_{QHtoHN})$ $X12(TWRI_{QHtoHN})$	……	……	……	……	……	\	\
Shandong	$X13(TWRA_{QHtoSD})$ $X14(TWRI_{QHtoSD})$	……	……	……	……	……	$X55(TWRA_{HNtoSD})$ $X56(TWRI_{HNtoSD})$	\
Area	**Qinghai**	**Gansu**	**Ningxia**	**Neimenggu**	**Shanxi**	**Shannxi**	**Henan**	**Shandong**
Qinghai	\	\	\	\	\	\	\	\
Gansu	$X57(TPRCOD_{QHtoGS})$ $X58(TPRNH4_{QHtoGS})$	\	\	\	\	\	\	\
Ningxia	$X59(TPRCOD_{QHtoNX})$ $X60(TPRNH4_{QHtoNX})$	……	\	\	\	\	\	\
Neimenggu	$X61(TPRCOD_{QHtoNMG})$ $X62(TPRNH4_{QHtoNMG})$	……	……	\	\	\	\	\
Shanxi	$X63(TPRCOD_{QHtoSX})$ $X64(TPRNH4_{QHtoSX})$	……	……	……	\	\	\	\
Shannxi	$X65(TPRCOD_{QHtoSHX})$ $X66(TPRNH4_{QHtoSHX})$	……	……	……	……	\	\	\
Henan	$X67(TPRCOD_{QHtoHN})$ $X68(TPRNH4_{QHtoHN})$	……	……	……	……	……	\	\
Shandong	$X69(TPRCOD_{QHtoSD})$ $X70(TPRNH4_{QHtoSD})$	……	……	……	……	……	$X55(TPRCOD_{HNtoSD})$ $X56(TPRNH4_{HNtoSD})$	\

Table S6 The average monthly discharge of reservoirs from 2015 to 2019(m^3/s)

Reservoirs	Longyangxia	Liujiaxia	Wanjiazhai	Xiaolangdi	Sanmenxia
201501	450	400	300	450	350
201502	450	300	350	550	450
201503	450	400	650	850	400
201504	450	500	250	800	500
201505	450	750	100	880	300
201506	450	700	200	850	300
201507	500	750	700	950	600
201508	450	700	450	400	500
201509	400	550	350	300	500
201510	400	500	300	300	400
201511	400	500	300	250	300
201512	400	300	300	250	350
201601	400	300	250	300	250
201602	400	300	300	450	250
201603	400	300	450	650	350
201604	400	450	200	600	200
201605	400	550	200	450	150
201606	400	700	250	300	200
201607	500	750	350	700	600
201608	450	750	350	600	400

201609	300	500	200	600	450
201610	300	500	200	500	300
201611	250	450	200	300	300
201612	250	300	200	200	300
201701	300	250	150	200	250
201702	300	250	300	350	300
201703	300	250	300	650	350
201704	350	450	300	550	350
201705	400	650	300	650	250
201706	400	600	400	600	300
201707	450	700	450	400	600
201708	450	700	350	400	600
201709	350	600	300	300	550
201710	350	600	300	300	550
201711	350	650	300	400	500
201712	400	300	400	400	350
201801	400	300	250	300	300
201802	400	300	300	400	400
201803	400	350	450	800	450
201804	500	600	350	1000	400
201805	550	850	150	950	500
201806	792	1000	400	1500	600
201807	750	1200	700	1500	1400
201808	650	1200	700	1500	1400
201809	600	750	600	1500	1600
201810	600	650	600	1200	1400
201811	650	660	500	650	750
201812	400	450	400	450	400
201901	400	350	300	350	460
201902	300	350	450	650	500
201903	450	450	550	850	550
201904	800	950	600	1200	700
201905	850	1000	450	1200	700
201906	875	1200	700	1500	800
201907	850	1200	850	2000	1200
201908	750	1200	850	950	1200
201909	700	750	700	1600	1200
201910	700	750	700	1200	1000
201911	700	700	500	700	750
201912	500	450	300	400	550