
Supplementary information for

**Millionfold accelerated AI Solver for 3D multi-physical
simulations of ultrapermeable membranes**

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1.Videos

Supplementary video 1 Velocity profiles in the x direction in 184 geometries of typical feed spacer predicted by the modified FNO-based method and calculated by CFD.

Supplementary video 2 Velocity profiles in the y direction in 184 geometries of typical feed spacer predicted by the modified FNO-based method and calculated by CFD.

Supplementary video 3 Velocity profiles in the z direction in 184 geometries of typical feed spacer predicted by the modified FNO-based method and calculated by CFD.

Supplementary video 4 Pressure profiles in 184 geometries of typical feed spacer predicted by the modified FNO-based method and calculated by CFD.

Supplementary video 5 Concentration profiles in 184 geometries of typical feed spacer predicted by the modified FNO-based method and calculated by CFD.

2. Figures

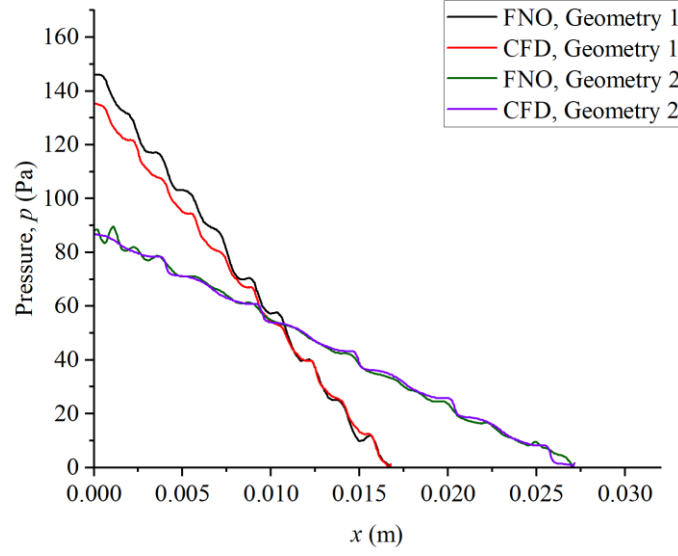


Fig. S1 The local pressure distribution along the transversal line of the membrane surface at $z = 0.5H, y = 0.25L_y, 0 \leq x \leq L_x$.

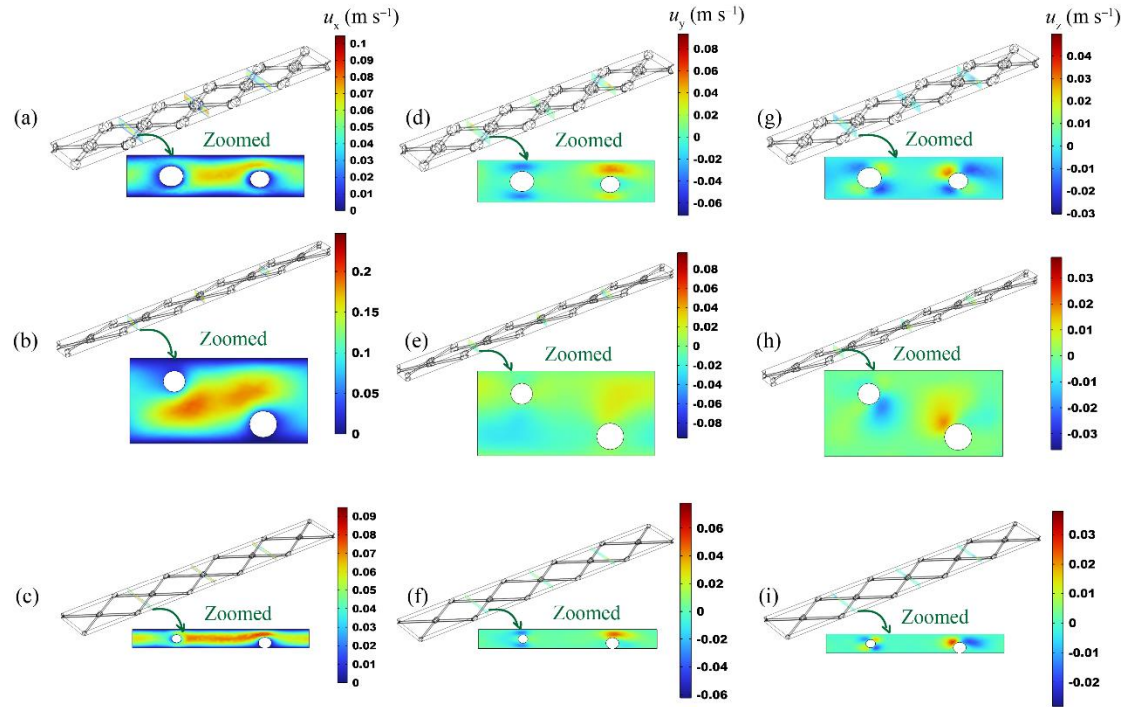


Fig. S2 The three components of velocity of the higher resolution dataset in 3 geometries of typical feed spacer predicted by the modified FNO-based method.

(a) - (c) are velocity in the x direction, (d) - (f) are velocity in the y direction, and (g) - (i) are velocity in the z direction.

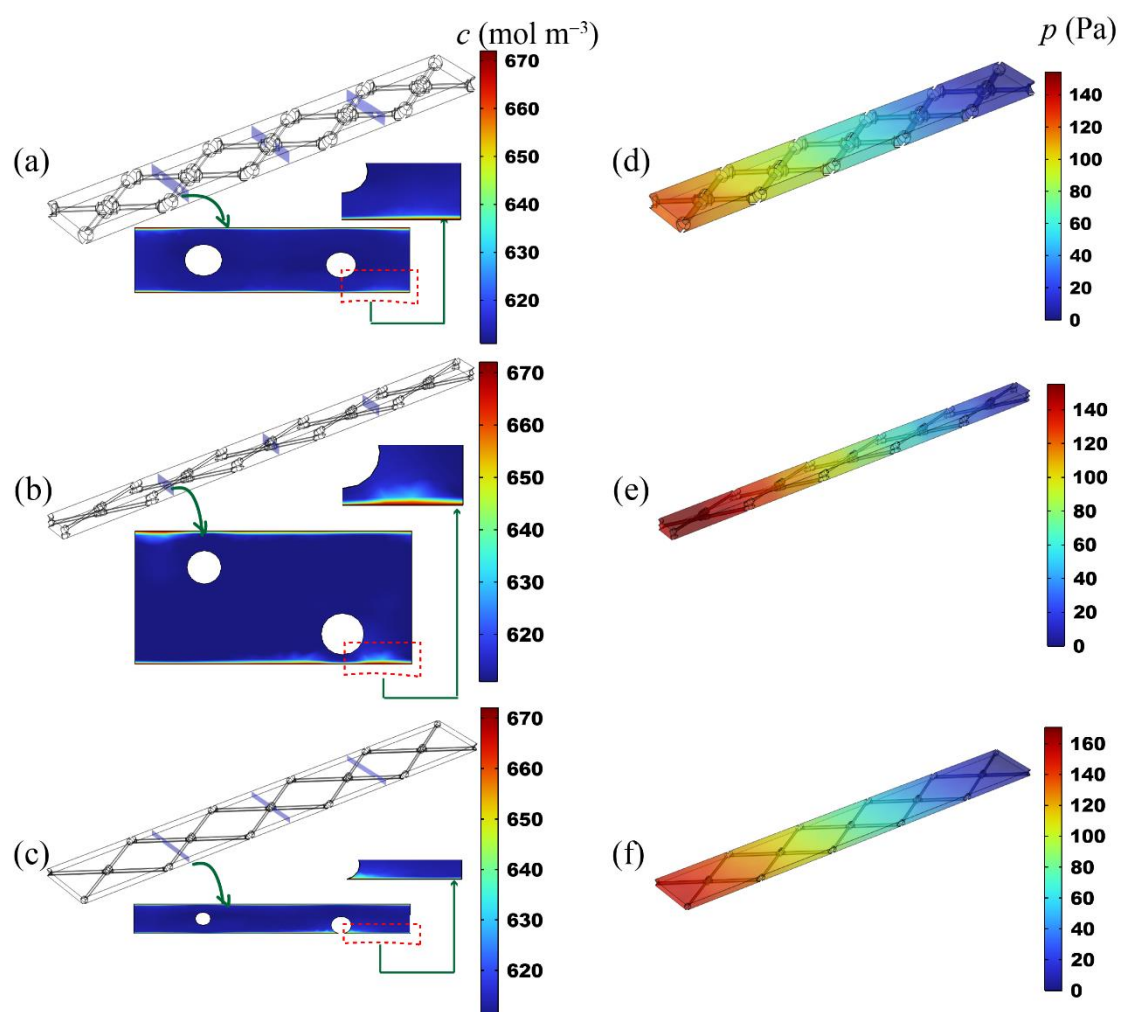


Fig. S3 Concentration and pressure of the higher resolution dataset in 3 geometries of typical feed spacer predicted by the modified FNO-based method. (a) - (c) are the results of concentration, and (d)-(f) are the results of pressure of the corresponding geometries.

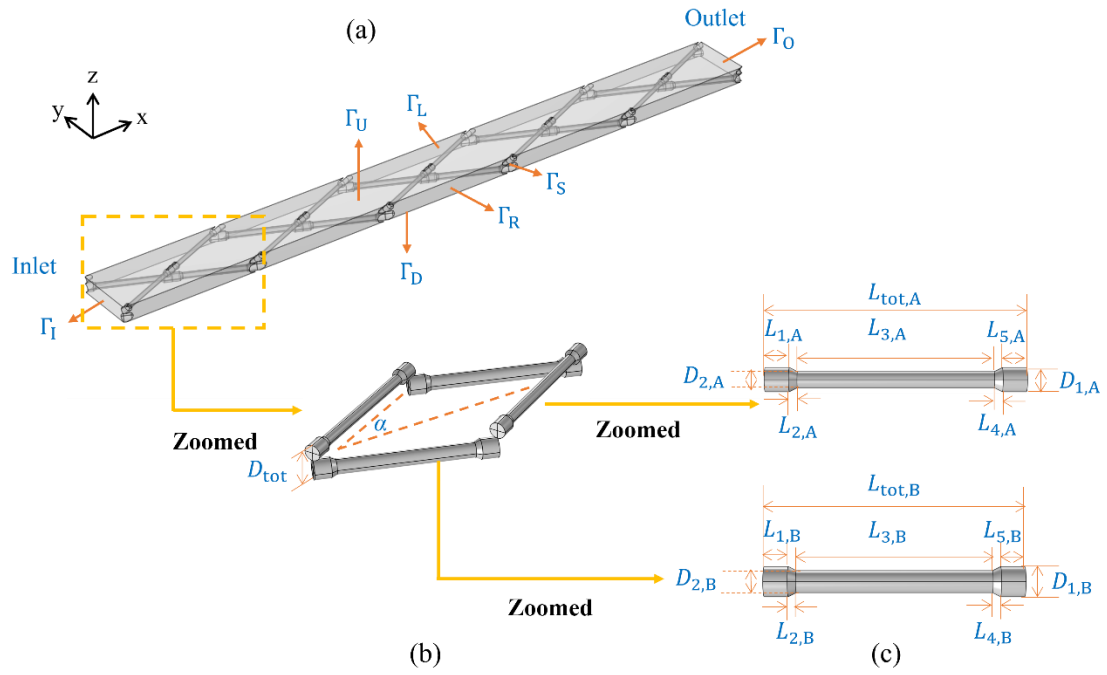


Fig. S4 Schematic diagram of 3D multi-physics modeling. (a) Computational domain of a CFD model; (b) A spacer unit; (c) Spacer filaments.

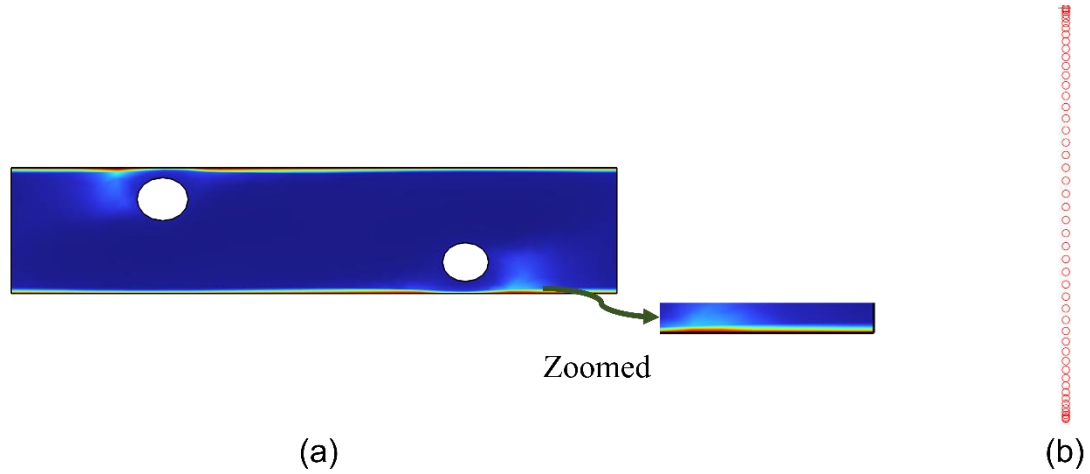


Fig. S5 Schematic diagram of concentration problem. (a) The distribution of concentration. (b) The interpolation strategy with logarithmic intervals.

3.Tables

Table S1 Comparison between velocity predicted by the modified FNO and CFD data.

Model	u_x			u_y			u_z		
	SSIM	RMSE	R^2	SSIM	RMSE	R^2	SSIM	RMSE	R^2
1	0.9914	0.0291	0.9869	0.9990	0.0111	0.9803	0.9968	0.0154	0.9693
2	0.9936	0.0278	0.9893	0.9997	0.0123	0.9793	0.9993	0.0141	0.9678
3	0.9709	0.0549	0.9369	0.9918	0.0344	0.9598	0.9941	0.0297	0.8817
4	0.9900	0.0246	0.9923	0.9995	0.0088	0.9892	0.9991	0.0094	0.9839
5	0.9925	0.0281	0.9865	0.9996	0.0145	0.9800	0.9983	0.0180	0.9577
6	0.9929	0.0250	0.9893	0.9993	0.0147	0.9862	0.9995	0.0162	0.9576
7	0.9862	0.0379	0.9734	0.9989	0.0177	0.9709	0.9942	0.0145	0.9696
8	0.9925	0.0368	0.9809	0.9991	0.0145	0.9807	0.9979	0.0163	0.9742
9	0.9884	0.0377	0.9561	0.9984	0.0197	0.9411	0.9951	0.0179	0.9419
10	0.9680	0.0490	0.9545	0.9946	0.0187	0.9454	0.9927	0.0174	0.9361
11	0.9919	0.0290	0.9859	0.9997	0.0113	0.9819	0.9988	0.0152	0.9588
12	0.9932	0.0230	0.9918	0.9987	0.0144	0.9864	0.9980	0.0138	0.9742
13	0.9936	0.0238	0.9879	0.9995	0.0096	0.9892	0.9987	0.0112	0.9808
14	0.9872	0.0311	0.9861	0.9998	0.0112	0.9695	0.9990	0.0118	0.9642
15	0.9958	0.0225	0.9909	0.9996	0.0143	0.9923	0.9994	0.0140	0.9629
16	0.9917	0.0246	0.9902	0.9990	0.0100	0.9902	0.9981	0.0084	0.9892
17	0.9948	0.0216	0.9930	0.9995	0.0129	0.9864	0.9987	0.0153	0.9796
18	0.9968	0.0228	0.9920	0.9998	0.0122	0.9782	0.9992	0.0202	0.9669
19	0.9875	0.0468	0.9632	0.9999	0.0241	0.9232	0.9995	0.0256	0.9132
20	0.9895	0.0243	0.9903	0.9995	0.0103	0.9874	0.9987	0.0116	0.9721
21	0.9938	0.0224	0.9903	0.9994	0.0146	0.9913	0.9996	0.0129	0.9545
22	0.9924	0.0266	0.9893	0.9992	0.0105	0.9880	0.9985	0.0110	0.9747
23	0.9933	0.0193	0.9931	0.9994	0.0087	0.9913	0.9980	0.0101	0.9860
24	0.9848	0.0542	0.9476	0.9963	0.0322	0.9669	0.9974	0.0314	0.8752
25	0.9855	0.0367	0.9766	0.9985	0.0177	0.9804	0.9995	0.0176	0.9330
26	0.9876	0.0291	0.9868	0.9982	0.0159	0.9840	0.9978	0.0129	0.9784
27	0.9908	0.0271	0.9886	0.9994	0.0139	0.9838	0.9982	0.0148	0.9796
28	0.9940	0.0193	0.9947	0.9997	0.0091	0.9910	0.9980	0.0143	0.9838
29	0.9919	0.0177	0.9952	0.9990	0.0115	0.9954	0.9987	0.0115	0.9848
30	0.9930	0.0251	0.9903	0.9994	0.0110	0.9887	0.9988	0.0105	0.9843
31	0.9905	0.0269	0.9869	0.9992	0.0144	0.9882	0.9990	0.0139	0.9682
32	0.9929	0.0287	0.9843	0.9993	0.0107	0.9832	0.9975	0.0135	0.9582
33	0.9848	0.0254	0.9812	0.9980	0.0140	0.9836	0.9943	0.0161	0.9711
34	0.9930	0.0255	0.9883	0.9995	0.0110	0.9870	0.9982	0.0133	0.9708
35	0.9811	0.0467	0.9627	0.9966	0.0290	0.9557	0.9971	0.0216	0.9360
36	0.9948	0.0175	0.9953	0.9996	0.0077	0.9941	0.9996	0.0076	0.9850

37	0.9937	0.0225	0.9917	0.9996	0.0121	0.9894	0.9976	0.0168	0.9779
38	0.9884	0.0344	0.9772	0.9996	0.0161	0.9624	0.9950	0.0147	0.9569
39	0.9953	0.0206	0.9928	0.9991	0.0132	0.9904	0.9992	0.0199	0.9442
40	0.9926	0.0255	0.9892	0.9994	0.0128	0.9861	0.9986	0.0162	0.9712
41	0.9868	0.0294	0.9869	0.9985	0.0143	0.9878	0.9961	0.0122	0.9824
42	0.9931	0.0257	0.9883	0.9991	0.0128	0.9843	0.9982	0.0129	0.9812
43	0.9918	0.0263	0.9887	0.9987	0.0128	0.9814	0.9980	0.0128	0.9807
44	0.9902	0.0236	0.9918	0.9960	0.0146	0.9933	0.9949	0.0130	0.9847
45	0.9871	0.0276	0.9838	0.9981	0.0133	0.9812	0.9964	0.0140	0.9708
46	0.9925	0.0223	0.9913	0.9994	0.0107	0.9886	0.9979	0.0115	0.9815
47	0.9859	0.0404	0.9735	0.9978	0.0217	0.9721	0.9971	0.0186	0.9547
48	0.9921	0.0249	0.9920	0.9997	0.0096	0.9878	0.9978	0.0153	0.9774
49	0.9917	0.0347	0.9811	0.9976	0.0217	0.9847	0.9983	0.0192	0.9635
50	0.9953	0.0236	0.9916	0.9996	0.0190	0.9770	0.9979	0.0255	0.9656
51	0.9937	0.0285	0.9861	0.9985	0.0176	0.9866	0.9988	0.0204	0.9292
52	0.9951	0.0268	0.9871	0.9996	0.0144	0.9638	0.9994	0.0140	0.9294
53	0.9925	0.0214	0.9936	0.9979	0.0149	0.9849	0.9973	0.0122	0.9840
54	0.9897	0.0358	0.9815	0.9977	0.0179	0.9748	0.9982	0.0137	0.9738
55	0.9874	0.0324	0.9782	0.9977	0.0217	0.9808	0.9965	0.0196	0.9498
56	0.9901	0.0203	0.9918	0.9989	0.0099	0.9934	0.9954	0.0100	0.9887
57	0.9876	0.0248	0.9910	0.9998	0.0102	0.9796	0.9994	0.0131	0.9722
58	0.9876	0.0344	0.9805	0.9990	0.0174	0.9796	0.9960	0.0169	0.9624
59	0.9944	0.0230	0.9888	0.9994	0.0098	0.9892	0.9988	0.0115	0.9787
60	0.9933	0.0221	0.9919	0.9992	0.0113	0.9889	0.9985	0.0108	0.9815
61	0.9831	0.0323	0.9684	0.9943	0.0205	0.9605	0.9921	0.0182	0.9701
62	0.9921	0.0366	0.9775	0.9997	0.0186	0.9623	0.9989	0.0240	0.9368
63	0.9825	0.0407	0.9706	0.9975	0.0250	0.9582	0.9926	0.0188	0.9534
64	0.9930	0.0323	0.9836	0.9993	0.0239	0.9788	0.9974	0.0403	0.8942
65	0.9851	0.0269	0.9860	0.9989	0.0124	0.9846	0.9965	0.0109	0.9804
66	0.9895	0.0320	0.9854	0.9992	0.0142	0.9872	0.9987	0.0149	0.9656
67	0.9961	0.0230	0.9903	0.9995	0.0175	0.9581	0.9998	0.0138	0.9383
68	0.9930	0.0293	0.9884	0.9996	0.0195	0.9789	0.9991	0.0186	0.9760
69	0.9868	0.0368	0.9761	0.9978	0.0243	0.9813	0.9960	0.0219	0.9414
70	0.9934	0.0236	0.9853	0.9990	0.0107	0.9855	0.9980	0.0122	0.9767
71	0.9906	0.0248	0.9904	0.9989	0.0126	0.9865	0.9982	0.0126	0.9830
72	0.9909	0.0282	0.9823	0.9987	0.0100	0.9825	0.9949	0.0145	0.9694
73	0.9936	0.0269	0.9886	0.9986	0.0132	0.9869	0.9982	0.0133	0.9732
74	0.9923	0.0245	0.9916	0.9992	0.0102	0.9887	0.9982	0.0115	0.9842
75	0.9929	0.0280	0.9847	0.9992	0.0114	0.9809	0.9974	0.0127	0.9692
76	0.9948	0.0194	0.9937	0.9997	0.0193	0.9759	0.9993	0.0230	0.9547
77	0.9896	0.0290	0.9846	0.9987	0.0131	0.9757	0.9961	0.0154	0.9647
78	0.9883	0.0324	0.9844	0.9990	0.0131	0.9726	0.9980	0.0180	0.9641
79	0.9941	0.0260	0.9868	0.9992	0.0134	0.9856	0.9972	0.0122	0.9787
80	0.9945	0.0240	0.9909	0.9970	0.0187	0.9886	0.9976	0.0176	0.9614

81	0.9875	0.0377	0.9729	0.9974	0.0216	0.9823	0.9972	0.0171	0.9512
82	0.9913	0.0332	0.9824	0.9995	0.0166	0.9821	0.9982	0.0201	0.9505
83	0.9954	0.0267	0.9868	0.9995	0.0156	0.9647	0.9989	0.0172	0.9170
84	0.9938	0.0368	0.9781	0.9996	0.0247	0.9665	0.9986	0.0397	0.9051
85	0.9911	0.0249	0.9842	0.9989	0.0127	0.9752	0.9971	0.0110	0.9780
86	0.9897	0.0310	0.9857	0.9990	0.0124	0.9844	0.9978	0.0146	0.9674
87	0.9945	0.0291	0.9844	0.9994	0.0130	0.9690	0.9994	0.0156	0.9140
88	0.9874	0.0237	0.9894	0.9988	0.0117	0.9870	0.9939	0.0111	0.9788
89	0.9897	0.0263	0.9888	0.9995	0.0102	0.9839	0.9969	0.0121	0.9741
90	0.9844	0.0327	0.9793	0.9984	0.0175	0.9634	0.9982	0.0110	0.9705
91	0.9898	0.0229	0.9920	0.9997	0.0091	0.9884	0.9990	0.0102	0.9782
92	0.9833	0.0369	0.9790	0.9977	0.0165	0.9733	0.9983	0.0139	0.9708
93	0.9884	0.0465	0.9537	0.9963	0.0294	0.9704	0.9991	0.0339	0.7598
94	0.9904	0.0334	0.9610	0.9976	0.0225	0.9374	0.9947	0.0174	0.9538
95	0.9881	0.0321	0.9863	0.9984	0.0158	0.9724	0.9991	0.0163	0.9577
96	0.9861	0.0301	0.9836	0.9989	0.0121	0.9845	0.9968	0.0111	0.9753
97	0.9939	0.0247	0.9903	0.9997	0.0123	0.9914	0.9993	0.0148	0.9715
98	0.9935	0.0221	0.9927	0.9995	0.0109	0.9862	0.9986	0.0124	0.9731
99	0.9880	0.0320	0.9852	0.9993	0.0148	0.9843	0.9986	0.0166	0.9766
100	0.9956	0.0203	0.9929	0.9998	0.0128	0.9843	0.9997	0.0143	0.9400
101	0.9948	0.0249	0.9901	0.9989	0.0129	0.9814	0.9979	0.0116	0.9816
102	0.9784	0.0522	0.9457	0.9977	0.0218	0.9708	0.9953	0.0194	0.9546
103	0.9909	0.0202	0.9939	0.9993	0.0083	0.9929	0.9979	0.0105	0.9883
104	0.9914	0.0268	0.9845	0.9991	0.0113	0.9861	0.9985	0.0120	0.9754
105	0.9767	0.0469	0.9600	0.9945	0.0299	0.9609	0.9966	0.0211	0.9297
106	0.9934	0.0229	0.9930	0.9989	0.0153	0.9765	0.9978	0.0154	0.9738
107	0.9912	0.0327	0.9803	0.9993	0.0152	0.9885	0.9975	0.0155	0.9702
108	0.9929	0.0300	0.9854	0.9998	0.0142	0.9802	0.9996	0.0159	0.9386
109	0.9954	0.0217	0.9921	0.9987	0.0134	0.9925	0.9993	0.0138	0.9715
110	0.9861	0.0280	0.9857	0.9994	0.0128	0.9772	0.9981	0.0093	0.9808
111	0.9841	0.0287	0.9869	0.9977	0.0182	0.9802	0.9967	0.0130	0.9833
112	0.9937	0.0290	0.9869	0.9996	0.0156	0.9758	0.9994	0.0170	0.9299
113	0.9896	0.0285	0.9883	0.9995	0.0165	0.9685	0.9988	0.0183	0.9647
114	0.9923	0.0237	0.9921	0.9989	0.0114	0.9870	0.9974	0.0129	0.9789
115	0.9934	0.0244	0.9912	0.9986	0.0128	0.9890	0.9981	0.0127	0.9773
116	0.9943	0.0254	0.9886	0.9991	0.0166	0.9873	0.9997	0.0192	0.8976
117	0.9947	0.0299	0.9870	0.9972	0.0174	0.9819	0.9985	0.0129	0.9776
118	0.9912	0.0296	0.9846	0.9980	0.0157	0.9837	0.9980	0.0151	0.9672
119	0.9926	0.0235	0.9904	0.9993	0.0106	0.9885	0.9984	0.0105	0.9847
120	0.9857	0.0462	0.9661	0.9993	0.0223	0.9637	0.9970	0.0180	0.9523
121	0.9861	0.0377	0.9779	0.9978	0.0261	0.9530	0.9967	0.0194	0.9673
122	0.9943	0.0256	0.9891	0.9992	0.0280	0.9069	0.9988	0.0274	0.8967
123	0.9857	0.0466	0.9670	0.9994	0.0224	0.9558	0.9973	0.0409	0.8822
124	0.9913	0.0267	0.9864	0.9987	0.0119	0.9825	0.9963	0.0118	0.9734

125	0.9854	0.0321	0.9867	0.9995	0.0134	0.9815	0.9975	0.0158	0.9649
126	0.9934	0.0265	0.9892	0.9999	0.0139	0.9741	0.9997	0.0142	0.9579
127	0.9777	0.0298	0.9816	0.9972	0.0119	0.9762	0.9965	0.0108	0.9748
128	0.9961	0.0195	0.9931	0.9996	0.0119	0.9899	0.9994	0.0194	0.9445
129	0.9867	0.0223	0.9890	0.9990	0.0105	0.9867	0.9948	0.0107	0.9809
130	0.9934	0.0270	0.9861	0.9997	0.0160	0.9593	0.9993	0.0184	0.9307
131	0.9927	0.0257	0.9907	0.9978	0.0192	0.9775	0.9982	0.0142	0.9755
132	0.9871	0.0317	0.9796	0.9991	0.0152	0.9790	0.9972	0.0166	0.9559
133	0.9911	0.0318	0.9871	0.9995	0.0157	0.9804	0.9987	0.0147	0.9737
134	0.9845	0.0448	0.9705	0.9957	0.0228	0.9441	0.9972	0.0179	0.9494
135	0.9920	0.0291	0.9841	0.9999	0.0159	0.9614	0.9997	0.0143	0.9566
136	0.9832	0.0284	0.9854	0.9988	0.0104	0.9831	0.9975	0.0098	0.9761
137	0.9859	0.0333	0.9837	0.9993	0.0190	0.9717	0.9985	0.0217	0.9595
138	0.9887	0.0338	0.9801	0.9997	0.0167	0.9718	0.9989	0.0196	0.9440
139	0.9927	0.0260	0.9834	0.9987	0.0114	0.9812	0.9958	0.0134	0.9676
140	0.9922	0.0354	0.9847	0.9995	0.0237	0.9623	0.9991	0.0258	0.9569
141	0.9902	0.0288	0.9810	0.9988	0.0135	0.9704	0.9978	0.0115	0.9662
142	0.9943	0.0243	0.9904	0.9990	0.0117	0.9917	0.9990	0.0118	0.9863
143	0.9913	0.0336	0.9739	0.9980	0.0164	0.9708	0.9976	0.0143	0.9594
144	0.9914	0.0227	0.9913	0.9996	0.0095	0.9898	0.9981	0.0108	0.9831
145	0.9861	0.0288	0.9873	0.9983	0.0136	0.9884	0.9965	0.0127	0.9826
146	0.9922	0.0228	0.9903	0.9992	0.0103	0.9908	0.9980	0.0126	0.9828
147	0.9937	0.0220	0.9915	0.9998	0.0106	0.9865	0.9991	0.0121	0.9804
148	0.9479	0.0590	0.9456	0.9974	0.0188	0.9446	0.9919	0.0184	0.9530
149	0.9880	0.0302	0.9827	0.9977	0.0166	0.9638	0.9979	0.0116	0.9689
150	0.9894	0.0325	0.9848	0.9863	0.0360	0.9660	0.9983	0.0213	0.9439
151	0.9942	0.0262	0.9901	0.9985	0.0157	0.9784	0.9979	0.0161	0.9753
152	0.9941	0.0147	0.9970	0.9994	0.0080	0.9952	0.9986	0.0092	0.9910
153	0.9848	0.0314	0.9768	0.9993	0.0151	0.9734	0.9930	0.0158	0.9631
154	0.9919	0.0359	0.9774	0.9986	0.0169	0.9792	0.9977	0.0184	0.9468
155	0.9922	0.0222	0.9924	0.9988	0.0108	0.9819	0.9987	0.0092	0.9860
156	0.9963	0.0195	0.9941	0.9997	0.0139	0.9800	0.9986	0.0163	0.9767
157	0.9855	0.0305	0.9791	0.9986	0.0146	0.9771	0.9939	0.0154	0.9712
158	0.9914	0.0338	0.9810	0.9985	0.0179	0.9804	0.9976	0.0227	0.9477
159	0.9936	0.0197	0.9943	0.9993	0.0104	0.9926	0.9983	0.0128	0.9833
160	0.9923	0.0258	0.9871	0.9988	0.0107	0.9855	0.9979	0.0116	0.9714
161	0.9931	0.0249	0.9911	0.9996	0.0098	0.9904	0.9981	0.0125	0.9836
162	0.9740	0.0515	0.9469	0.9932	0.0334	0.9228	0.9929	0.0274	0.8928
163	0.9928	0.0250	0.9903	0.9987	0.0110	0.9842	0.9975	0.0121	0.9804
164	0.9662	0.0559	0.9609	0.9993	0.0230	0.9598	0.9982	0.0262	0.9022
165	0.9932	0.0209	0.9917	0.9991	0.0092	0.9905	0.9971	0.0104	0.9834
166	0.9948	0.0174	0.9961	0.9990	0.0090	0.9943	0.9982	0.0087	0.9931
167	0.9912	0.0285	0.9864	0.9977	0.0189	0.9806	0.9980	0.0143	0.9717
168	0.9913	0.0329	0.9810	0.9985	0.0233	0.9695	0.9994	0.0202	0.9065

169	0.9750	0.0357	0.9809	0.9977	0.0195	0.9484	0.9959	0.0143	0.9729
170	0.9941	0.0281	0.9813	0.9996	0.0113	0.9804	0.9967	0.0122	0.9708
171	0.9937	0.0215	0.9928	0.9994	0.0107	0.9919	0.9982	0.0105	0.9825
172	0.9866	0.0472	0.9508	0.9986	0.0244	0.9700	0.9972	0.0270	0.9356
173	0.9860	0.0269	0.9859	0.9988	0.0153	0.9835	0.9946	0.0149	0.9749
174	0.9828	0.0318	0.9843	0.9996	0.0105	0.9801	0.9977	0.0126	0.9599
175	0.9885	0.0431	0.9678	0.9996	0.0172	0.9660	0.9989	0.0217	0.8867
176	0.9918	0.0312	0.9833	0.9997	0.0204	0.9721	0.9983	0.0255	0.9398
177	0.9941	0.0217	0.9927	0.9984	0.0121	0.9931	0.9964	0.0125	0.9864
178	0.9837	0.0415	0.9652	0.9975	0.0274	0.9333	0.9952	0.0272	0.9207
179	0.9568	0.0523	0.9544	0.9929	0.0289	0.9685	0.9908	0.0271	0.9362
180	0.9955	0.0193	0.9949	0.9986	0.0132	0.9850	0.9983	0.0128	0.9851
181	0.9937	0.0309	0.9851	0.9992	0.0165	0.9791	0.9986	0.0161	0.9749
182	0.9933	0.0253	0.9885	0.9998	0.0118	0.9827	0.9992	0.0178	0.9641
183	0.9941	0.0248	0.9895	0.9996	0.0166	0.9641	0.9980	0.0294	0.9422
184	0.9942	0.0207	0.9923	0.9998	0.0124	0.9839	0.9994	0.0168	0.9531

Table S2 Comparison between pressure and concentration predicted by the modified FNO and CFD data.

Model	p			c		
	SSIM	RMSE	R^2	SSIM	RMSE	R^2
1	0.9990	0.0159	0.9963	0.9865	0.0038	0.9897
2	0.9728	0.0556	0.9583	0.9912	0.0026	0.9971
3	0.9970	0.0244	0.9909	0.9894	0.0043	0.9961
4	0.9998	0.0155	0.9968	0.9915	0.0025	0.9958
5	0.9972	0.0278	0.9889	0.9883	0.0029	0.9931
6	0.9939	0.0315	0.9844	0.9882	0.0036	0.9970
7	0.9983	0.0201	0.9946	0.9909	0.0297	0.9929
8	0.9974	0.0392	0.9779	0.9919	0.0027	0.9933
9	0.9803	0.0821	0.9120	0.9915	0.0378	0.9877
10	0.9900	0.0932	0.8185	0.9874	0.0043	0.9942
11	0.9964	0.0332	0.9850	0.9881	0.0034	0.9967
12	0.9937	0.0421	0.9703	0.9928	0.0024	0.9988
13	0.9994	0.0088	0.9990	0.9925	0.0026	0.9941
14	0.9945	0.0363	0.9838	0.9911	0.0025	0.9940
15	0.9988	0.0171	0.9952	0.9923	0.0025	0.9984
16	0.9982	0.0117	0.9967	0.9906	0.0029	0.9984
17	0.9865	0.0802	0.9129	0.9915	0.0026	0.9976
18	0.9901	0.0607	0.9498	0.9934	0.0033	0.9988
19	0.9827	0.0642	0.9435	0.9904	0.0038	0.9859
20	0.9981	0.0314	0.9871	0.9942	0.0027	0.9939
21	0.9997	0.0110	0.9978	0.9932	0.0028	0.9993
22	0.9997	0.0085	0.9989	0.9866	0.0033	0.9944
23	0.9983	0.0143	0.9972	0.9878	0.0212	0.9964
24	0.9964	0.0485	0.9513	0.9857	0.0041	0.9988
25	0.9984	0.0182	0.9949	0.9918	0.0035	0.9979
26	0.9990	0.0112	0.9980	0.9897	0.0037	0.9975
27	0.9993	0.0151	0.9972	0.9911	0.0027	0.9953
28	0.9972	0.0604	0.9492	0.9940	0.0029	0.9965
29	0.9984	0.0154	0.9963	0.9917	0.0021	0.9995
30	0.9997	0.0141	0.9971	0.9899	0.0034	0.9977
31	0.9968	0.0344	0.9830	0.9922	0.0031	0.9957
32	0.9983	0.0180	0.9946	0.9851	0.0027	0.9938
33	0.9984	0.0378	0.9814	0.9808	0.0041	0.9875
34	0.9992	0.0163	0.9965	0.9886	0.0032	0.9961
35	0.9983	0.0206	0.9919	0.9894	0.0039	0.9980
36	0.9996	0.0099	0.9985	0.9940	0.0021	0.9990
37	0.9817	0.0511	0.9598	0.9949	0.0026	0.9983
38	0.9837	0.0811	0.9156	0.9827	0.0283	0.9936

39	0.9961	0.0378	0.9818	0.9952	0.0027	0.9994
40	0.9987	0.0162	0.9962	0.9870	0.0030	0.9968
41	0.9995	0.0104	0.9975	0.9897	0.0033	0.9985
42	0.9937	0.0313	0.9864	0.9797	0.0033	0.9908
43	0.9916	0.0761	0.9193	0.9843	0.0042	0.9952
44	0.9996	0.0081	0.9988	0.9902	0.0023	0.9995
45	0.9993	0.0104	0.9986	0.9902	0.0032	0.9926
46	0.9997	0.0061	0.9994	0.9888	0.0027	0.9958
47	0.9986	0.0150	0.9958	0.9882	0.0043	0.9975
48	0.9938	0.0395	0.9803	0.9886	0.0029	0.9967
49	0.9996	0.0117	0.9975	0.9796	0.0040	0.9969
50	0.9993	0.0198	0.9947	0.9940	0.0031	0.9992
51	0.9946	0.0412	0.9730	0.9925	0.0029	0.9984
52	0.9980	0.0183	0.9952	0.9914	0.0034	0.9986
53	0.9968	0.0285	0.9876	0.9912	0.0022	0.9991
54	0.9978	0.0268	0.9865	0.9882	0.0039	0.9975
55	0.9827	0.0479	0.9673	0.9861	0.0039	0.9911
56	0.9992	0.0132	0.9977	0.9902	0.0027	0.9959
57	0.9961	0.0271	0.9909	0.9892	0.0023	0.9960
58	0.9958	0.0443	0.9714	0.9890	0.0364	0.9887
59	0.9995	0.0095	0.9988	0.9862	0.0026	0.9941
60	0.9927	0.0417	0.9758	0.9922	0.0030	0.9948
61	0.9976	0.0180	0.9957	0.9719	0.0051	0.9805
62	0.9998	0.0104	0.9985	0.9899	0.0037	0.9953
63	0.9972	0.0366	0.9824	0.9802	0.0403	0.9868
64	0.9851	0.0783	0.9134	0.9956	0.0031	0.9990
65	0.9993	0.0152	0.9968	0.9870	0.0038	0.9925
66	0.9892	0.0662	0.9388	0.9904	0.0029	0.9948
67	0.9933	0.0340	0.9822	0.9940	0.0025	0.9994
68	0.9978	0.0189	0.9947	0.9872	0.0031	0.9987
69	0.9912	0.0686	0.9184	0.9878	0.0035	0.9980
70	0.9994	0.0078	0.9991	0.9871	0.0035	0.9898
71	0.9942	0.0301	0.9840	0.9913	0.0035	0.9957
72	0.9914	0.0445	0.9755	0.9920	0.0244	0.9953
73	0.9988	0.0205	0.9933	0.9881	0.0034	0.9973
74	0.9994	0.0149	0.9967	0.9890	0.0032	0.9974
75	0.9995	0.0191	0.9952	0.9896	0.0036	0.9948
76	0.9996	0.0101	0.9986	0.9951	0.0025	0.9994
77	0.9974	0.0192	0.9946	0.9896	0.0031	0.9932
78	0.9816	0.0515	0.9654	0.9900	0.0267	0.9943
79	0.9992	0.0128	0.9978	0.9890	0.0027	0.9967
80	0.9970	0.0255	0.9884	0.9912	0.0029	0.9991
81	0.9986	0.0257	0.9889	0.9907	0.0039	0.9978
82	0.9970	0.0241	0.9919	0.9892	0.0032	0.9921

83	0.9829	0.0626	0.9415	0.9892	0.0032	0.9984
84	0.9945	0.0398	0.9781	0.9909	0.0042	0.9977
85	0.9940	0.0360	0.9833	0.9853	0.0031	0.9921
86	0.9991	0.0106	0.9985	0.9896	0.0027	0.9971
87	0.9939	0.0292	0.9871	0.9940	0.0030	0.9988
88	0.9961	0.0290	0.9887	0.9881	0.0030	0.9924
89	0.9944	0.0407	0.9788	0.9884	0.0023	0.9957
90	0.9990	0.0164	0.9961	0.9890	0.0036	0.9962
91	0.9992	0.0249	0.9914	0.9887	0.0028	0.9928
92	0.9940	0.0379	0.9666	0.9850	0.0040	0.9964
93	0.9972	0.0384	0.9702	0.9891	0.0042	0.9982
94	0.9806	0.0507	0.9649	0.9812	0.0045	0.9811
95	0.9967	0.0283	0.9902	0.9902	0.0027	0.9929
96	0.9983	0.0145	0.9971	0.9902	0.0032	0.9962
97	0.9969	0.0231	0.9919	0.9924	0.0028	0.9978
98	0.9973	0.0222	0.9929	0.9924	0.0024	0.9986
99	0.9998	0.0116	0.9982	0.9886	0.0034	0.9972
100	0.9952	0.0276	0.9889	0.9918	0.0023	0.9996
101	0.9944	0.0457	0.9693	0.9841	0.0034	0.9964
102	0.9981	0.0264	0.9906	0.9850	0.0038	0.9885
103	0.9982	0.0174	0.9951	0.9931	0.0026	0.9971
104	0.9986	0.0148	0.9970	0.9935	0.0028	0.9931
105	0.9985	0.0244	0.9911	0.9852	0.0043	0.9961
106	0.9838	0.0962	0.8679	0.9927	0.0031	0.9979
107	0.9909	0.0556	0.9573	0.9899	0.0029	0.9902
108	0.9968	0.0296	0.9872	0.9857	0.0034	0.9947
109	0.9998	0.0108	0.9981	0.9883	0.0030	0.9986
110	0.9985	0.0163	0.9962	0.9895	0.0035	0.9921
111	0.9982	0.0186	0.9934	0.9900	0.0039	0.9982
112	0.9978	0.0164	0.9957	0.9906	0.0030	0.9987
113	0.9994	0.0129	0.9978	0.9843	0.0034	0.9898
114	0.9895	0.0350	0.9815	0.9855	0.0032	0.9973
115	0.9973	0.0233	0.9916	0.9929	0.0030	0.9972
116	0.9964	0.0384	0.9716	0.9867	0.0042	0.9985
117	0.9978	0.0283	0.9882	0.9867	0.0038	0.9967
118	0.9904	0.0556	0.9481	0.9907	0.0032	0.9963
119	0.9976	0.0253	0.9846	0.9907	0.0039	0.9974
120	0.9984	0.0147	0.9960	0.9833	0.0345	0.9903
121	0.9744	0.0451	0.9424	0.9862	0.0032	0.9981
122	0.9153	0.0976	0.8715	0.9933	0.0029	0.9988
123	0.9967	0.0232	0.9931	0.9905	0.0043	0.9958
124	0.9801	0.0486	0.9692	0.9907	0.0024	0.9955
125	0.9998	0.0098	0.9988	0.9897	0.0028	0.9940
126	0.9973	0.0241	0.9925	0.9900	0.0302	0.9924

127	0.9769	0.0556	0.9552	0.9765	0.0041	0.9886
128	0.9956	0.0319	0.9867	0.9867	0.0035	0.9984
129	0.9970	0.0220	0.9935	0.9897	0.0029	0.9935
130	0.9818	0.0805	0.9142	0.9904	0.0027	0.9943
131	0.9861	0.0955	0.8695	0.9909	0.0032	0.9976
132	0.9860	0.0821	0.9069	0.9889	0.0031	0.9965
133	0.9996	0.0129	0.9979	0.9895	0.0031	0.9965
134	0.9916	0.0939	0.8555	0.9840	0.0058	0.9936
135	0.9997	0.0167	0.9964	0.9922	0.0028	0.9924
136	0.9916	0.0337	0.9838	0.9873	0.0036	0.9953
137	0.9926	0.0444	0.9726	0.9870	0.0033	0.9966
138	0.9943	0.0310	0.9869	0.9896	0.0031	0.9907
139	0.9916	0.0423	0.9769	0.9915	0.0288	0.9935
140	0.9820	0.0482	0.9642	0.9897	0.0030	0.9987
141	0.9979	0.0218	0.9935	0.9871	0.0042	0.9877
142	0.9997	0.0121	0.9978	0.9902	0.0026	0.9981
143	0.9931	0.0445	0.9722	0.9892	0.0039	0.9875
144	0.9984	0.0169	0.9964	0.9910	0.0026	0.9942
145	0.9990	0.0144	0.9953	0.9911	0.0035	0.9979
146	0.9938	0.0463	0.9723	0.9903	0.0030	0.9941
147	0.9891	0.0396	0.9788	0.9898	0.0024	0.9941
148	0.9982	0.0167	0.9939	0.9766	0.0049	0.9958
149	0.9971	0.0410	0.9660	0.9844	0.0049	0.9916
150	0.9985	0.0241	0.9915	0.9910	0.0026	0.9992
151	0.9970	0.0302	0.9887	0.9903	0.0031	0.9907
152	0.9996	0.0137	0.9970	0.9926	0.0022	0.9994
153	0.9971	0.0334	0.9860	0.9884	0.0267	0.9941
154	0.9902	0.0573	0.9356	0.9886	0.0032	0.9964
155	0.9993	0.0155	0.9949	0.9910	0.0031	0.9984
156	0.9917	0.0371	0.9828	0.9925	0.0032	0.9979
157	0.9993	0.0169	0.9961	0.9905	0.0037	0.9867
158	0.9933	0.0384	0.9803	0.9896	0.0033	0.9906
159	0.9841	0.0494	0.9653	0.9936	0.0023	0.9991
160	0.9996	0.0079	0.9990	0.9915	0.0035	0.9916
161	0.9972	0.0250	0.9916	0.9932	0.0024	0.9964
162	0.9968	0.0217	0.9934	0.9860	0.0045	0.9820
163	0.9943	0.0339	0.9774	0.9875	0.0040	0.9961
164	0.9915	0.0692	0.9428	0.9734	0.0526	0.9791
165	0.9931	0.0490	0.9656	0.9928	0.0023	0.9955
166	0.9994	0.0114	0.9980	0.9943	0.0020	0.9993
167	0.9964	0.0199	0.9925	0.9905	0.0032	0.9975
168	0.9965	0.0297	0.9853	0.9860	0.0043	0.9973
169	0.9919	0.0304	0.9800	0.9815	0.0048	0.9961
170	0.9922	0.0457	0.9735	0.9903	0.0029	0.9920

171	0.9923	0.0378	0.9804	0.9942	0.0025	0.9981
172	0.9975	0.0291	0.9885	0.9831	0.0049	0.9874
173	0.9980	0.0305	0.9877	0.9825	0.0034	0.9924
174	0.9997	0.0059	0.9995	0.9899	0.0263	0.9945
175	0.9971	0.0279	0.9879	0.9976	0.0034	0.9992
176	0.9924	0.0482	0.9677	0.9939	0.0034	0.9933
177	0.9986	0.0134	0.9951	0.9887	0.0029	0.9978
178	0.9951	0.0665	0.9434	0.9835	0.0043	0.9879
179	0.9051	0.0987	0.8055	0.9830	0.0040	0.9982
180	0.9923	0.0591	0.9348	0.9905	0.0035	0.9982
181	0.9962	0.0312	0.9873	0.9929	0.0030	0.9909
182	0.9997	0.0081	0.9992	0.9950	0.0026	0.9962
183	0.9888	0.0677	0.9400	0.9956	0.0027	0.9981
184	0.9983	0.0178	0.9954	0.9907	0.0024	0.9995

Table S3 Comparison between velocity predicted by the modified FNO and CFD data in the higher resolution dataset.

Model	u_x			u_y			u_z		
	SSIM	RMSE	R^2	SSIM	RMSE	R^2	SSIM	RMSE	R^2
1	0.9796	0.0717	0.9211	0.9890	0.0309	0.9084	0.9949	0.0325	0.9011
2	0.9713	0.0575	0.9556	0.9952	0.0384	0.8933	0.9964	0.0316	0.9086
3	0.9755	0.0548	0.9483	0.9987	0.0199	0.9352	0.9968	0.0227	0.9306
4	0.9709	0.0657	0.9230	0.9984	0.0327	0.8823	0.9981	0.0311	0.8332
5	0.9690	0.0784	0.8637	0.9978	0.0331	0.8377	0.9946	0.0348	0.7684
6	0.9514	0.1190	0.7392	0.9933	0.0791	0.6082	0.9962	0.0494	0.6540
7	0.9666	0.0772	0.8974	0.9973	0.0446	0.8269	0.9968	0.0393	0.8276
8	0.9370	0.0878	0.8787	0.9841	0.0573	0.8023	0.9939	0.0388	0.8210
9	0.9688	0.0689	0.9094	0.9921	0.0365	0.8730	0.9948	0.0345	0.8625
10	0.9641	0.0700	0.9151	0.9938	0.0347	0.8479	0.9937	0.0320	0.8762

Table S4 Comparison between pressure and concentration predicted by the modified FNO and CFD data in the higher resolution dataset.

Model	p			c		
	SSIM	RMSE	R^2	SSIM	RMSE	R^2
1	0.9817	0.0473	0.9646	0.9848	0.0046	0.9789
2	0.9962	0.0612	0.9398	0.9681	0.0096	0.9854
3	0.9934	0.0280	0.9883	0.9613	0.0064	0.9708
4	0.9901	0.0425	0.9726	0.9851	0.0041	0.9986
5	0.9720	0.0921	0.8879	0.9761	0.0812	0.9431
6	0.9961	0.0318	0.9854	0.9686	0.0171	0.9792
7	0.9835	0.0601	0.9468	0.9792	0.0065	0.9836
8	0.9822	0.0535	0.9217	0.9850	0.0089	0.9895
9	0.9858	0.0798	0.8977	0.9706	0.0063	0.9770
10	0.9437	0.1262	0.6943	0.9536	0.0089	0.9784