ICSC 2019

Core Competence Enhanced by MBD

IDAJ CAE Solution Conference

2019/11/21

基于*CONVERGE*的柴油机*Urea-SCR*系统的数值模拟与结构优化

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目 录

SCR技术应用的背景

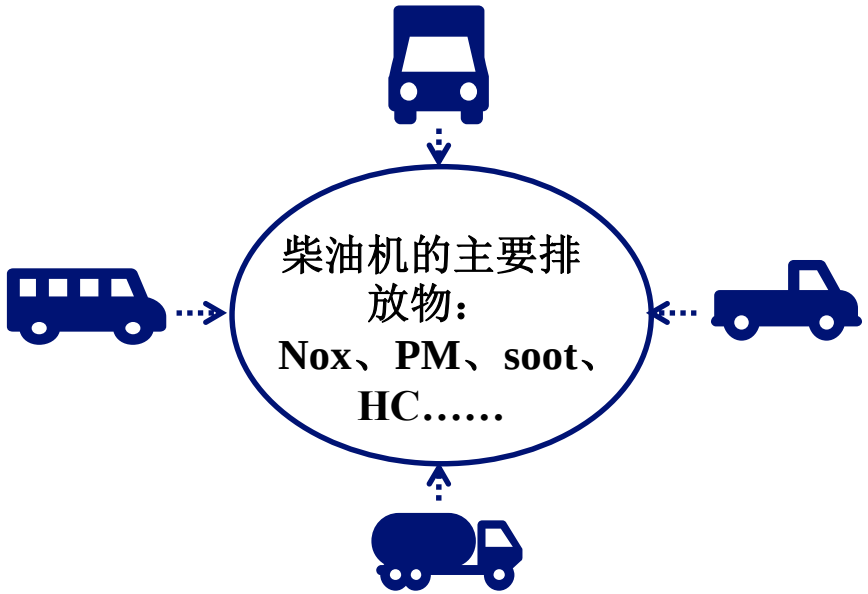
重型柴油车污染物排放限值及测量方法

（中国第六阶段）

Limits and measurement methods for emissions from diesel fuelled heavy-duty vehicles (CHINA VI)

（发布稿）

2018年6月22号发布，2020年1月1日全面实施



发动机类型	CO (mg/kWh)	THC (mg/kWh)	NO_X (mg/kWh)	PN[2] (#/kWh)
压燃式	6000	—	690	1.2×10^{12}
点燃式	6000	240（LPG） 750（NG）	690	—
双燃料	6000	1.5×WHTC 限值	690	1.2×10^{12}

(1) 应在同一次试验中同时测量 CO_2 并同时记录。

(2) PN 限值从 6b 阶段开始实施。

试验	CO (mg/kWh)	THC (mg/kWh)	NMHC (mg/kWh)	CH_4 (mg/kWh)	NO_X (mg/kWh)	NH_3 (ppm)	PM (mg/kWh)	PN (#/kWh)
WHSC 工况 (CI[1])	1500	130	—	—	400	10	10	8.0×10^{11}
WHTC 工况 (CI[1])	4000	160	—	—	460	10	10	6.0×10^{11}
WHTC 工况 (PI[2])	4000	—	160	500	460	10	10	6.0×10^{11}

(1)CI=压燃式发动机

(2)PI=点燃式发动机

Urea-SCR系统工作原理

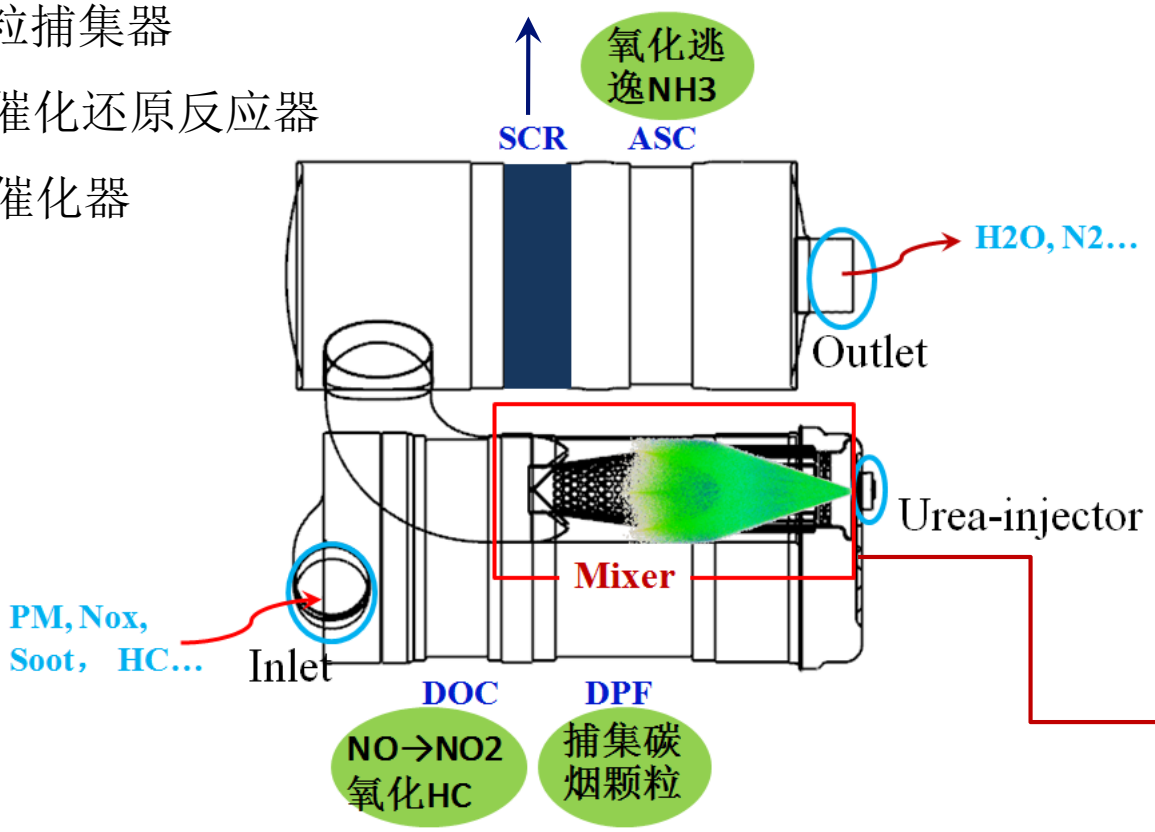
DOC：柴油氧化催化器

DPF：柴油颗粒捕集器

SCR：选择性催化还原反应器

ASC：氨逃逸催化器

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$$
$$2NH_3 + NO + NO_2 \rightarrow 2N_2 + 3H_2O$$
$$8NH_3 + 6NO_2 \rightarrow 7N_2 + 12H_2O$$



32.5%的尿素水溶液

与废气混合，换热，水蒸发

固体尿素

继续受热分解

直接热解法

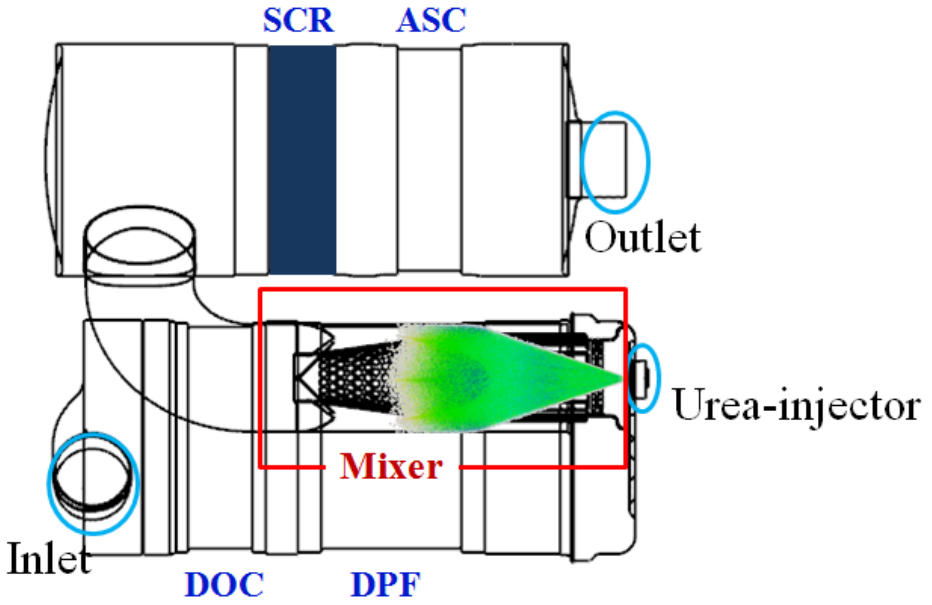
NH_3
HNCO

化学动力学法

NH_3
HNCO
Biuret
CYA
Ammelide
……

研究热点与难点

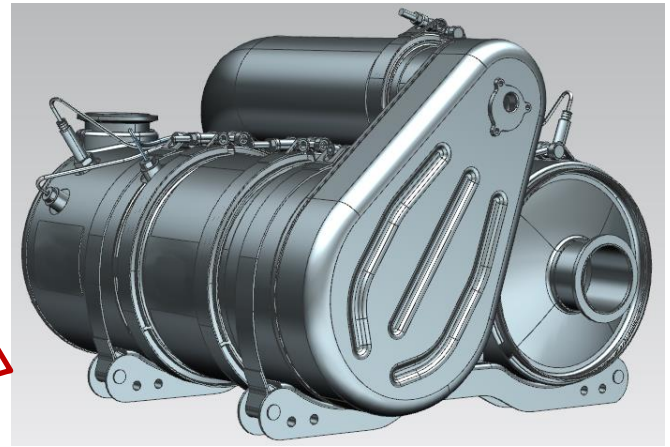
- 尿素详细分解机理
- 如何在有限的停留时间内提高尿素分解率
- 选用合适的催化剂
- NH_3/NO_x转化效率



基于CONVERGE的数值模拟

□ 模型的建立

简化前



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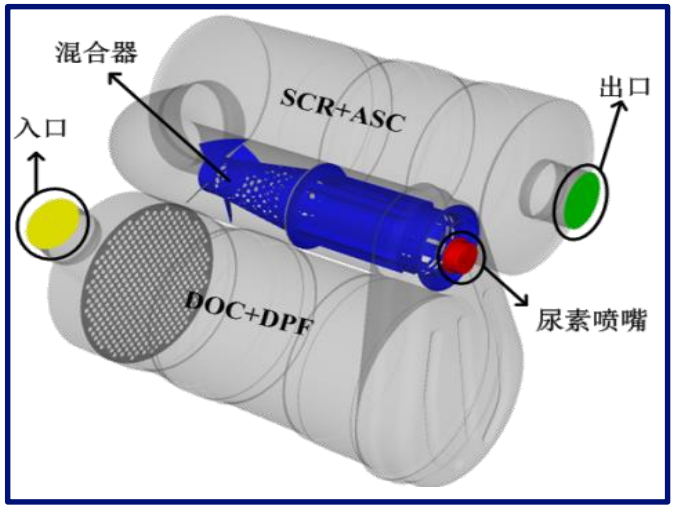


物理模型	
蒸发模型	Frossling model with boiling model
尿素分解模型	Detailed decomposition
喷雾与壁面交互模型	Kuhnke model
喷雾破碎模型	TAB
液滴分布	Rosin-Rammler
湍流模型	RNG k-ε

边界条件设置

网格划分

求解器设置.....

Reaction	Ai(s^{-1})	Ei(kJ • mol^{-1})
(R1) $urea \rightarrow NH_4^+ + NCO^-$	8.5×10^6	84
(R2) $NH_4^+ \rightarrow NH_3(g) + H^+$	1.50×10^2	40
(R3) $NCO^- + H^+ \rightarrow HNCO(g)$	6.57×10^2	10
(R4) $urea + NCO^- + H^+ \rightarrow biuret$	7.87×10^{14}	115
(R5) $biuret \rightarrow urea + NCO^- + H^+$	1.50×10^{24}	250
(R6) $biuret + NCO^- + H^+ \rightarrow cya + NH_3(g)$	2.81×10^{18}	150
(R7) $cya \rightarrow 3NCO^- + 3H^+$	1.50×10^{19}	260
(R8) $cya + NCO^- + H^+ \rightarrow ammelide + CO_2$	3.48×10^5	35
(R9) $ammelide \rightarrow 2NCO^- + 2H^+ + HCN(g) + NH(g)$	6.00×10^{14}	220
(R10) $urea(aq) \rightarrow NH_4^+ + NCO^-$	1.20×10^8	84
(R11) $NCO^- + H^+ + H_2O(g) \rightarrow NH_3 + CO_2(g)$	5.62×10^9	59
(R12) $urea(aq) + NCO^- + H^+ \rightarrow biuret$	3.93×10^{14}	115

Ebrahimian（图卢兹大学）等人提出的包含**12步化学反应的尿素详细分解机理**：

前9步反应主要描述了尿素在干燥介质中的热分解；

后3步反应主要描述了尿素在溶液中的热分解；

同时考虑了**biuret、CYA和ammelide**三种主要副产物的生成。

沉积物：尿素结晶、biuret、CYA和ammelide

Ebrahimian V, Nicolle A, Habchi C. Detailed modeling of the evaporation and thermal decomposition of urea-water solution in SCR systems[J]. AIChE Journal, 2012, 58(7): 1998-2009.

基础网格尺寸：
8mm

基于速度变化率自适应加密(AMR)

喷嘴

混合器

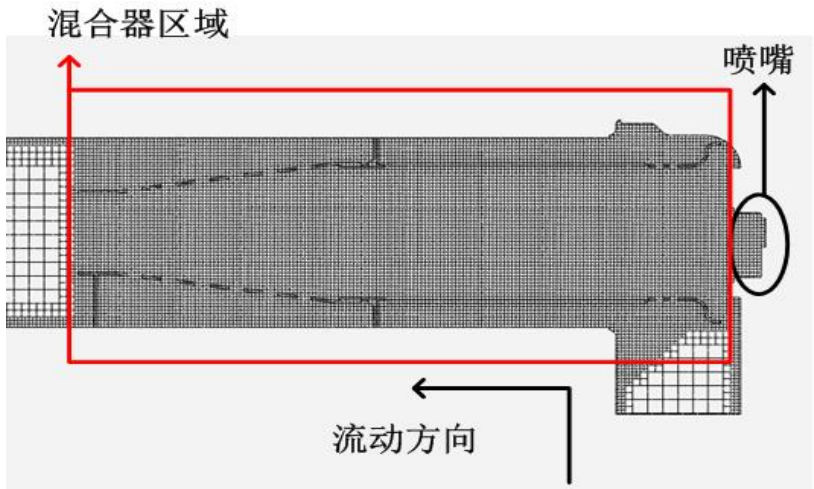
混合器管段

Fixed embedding

尿素喷束区域：圆锥型网格加密
喷嘴网格加密

混合管区域：圆柱型网格加密

SCR入口管段：boundary网格加密



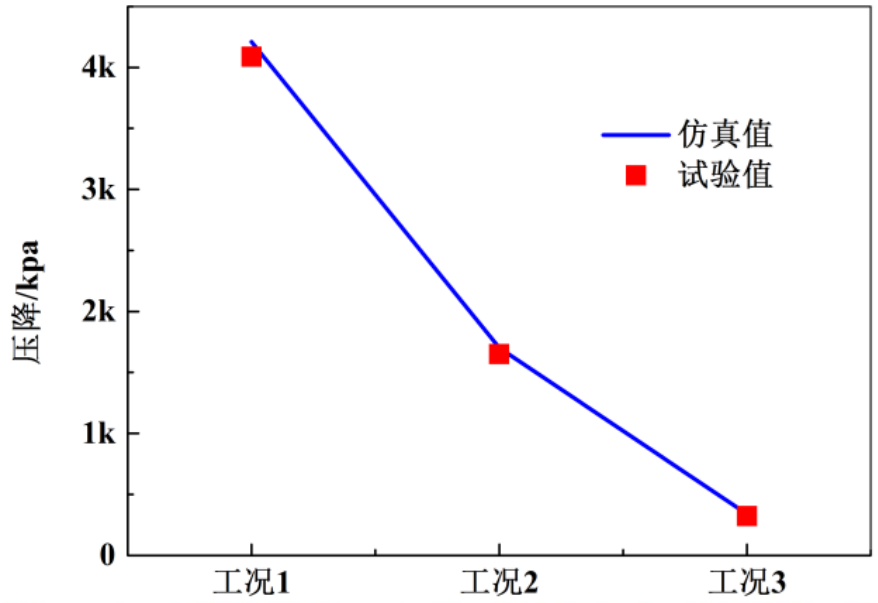
最小网格尺寸：**2mm**

最大网格总数：**976314个**

基于CONVERGE的数值模拟

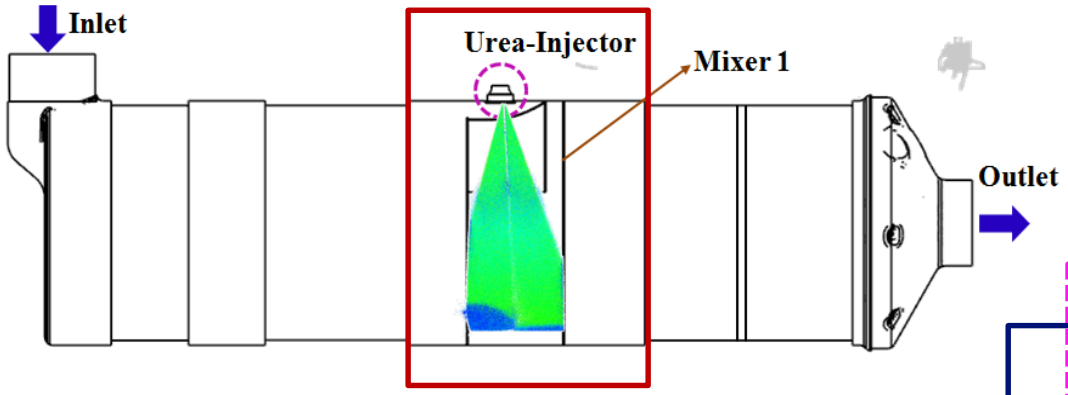
模型的验证

工况	转速 (r/min)	扭矩 （NM）	功率 （kw）	燃油消耗率	排气温度 (K)	排气流量 （kg/h）
1	2200	668.6	154	32.91	773	763.01
2	1800	513.6	96.82	18.93	626	525.93
3	1800	86.1	16.22	4.87	523	233.17

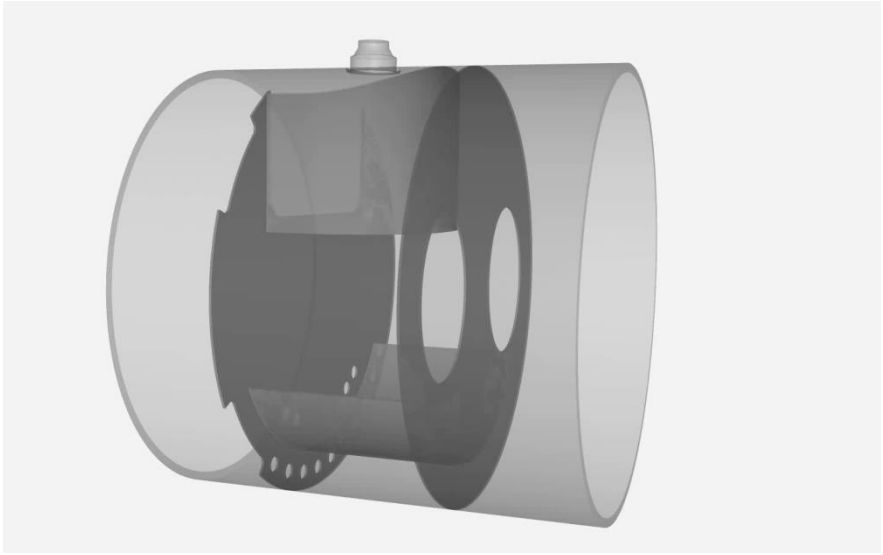


对比试验数据与仿真结果：

三个工况点压降误差均小于5%



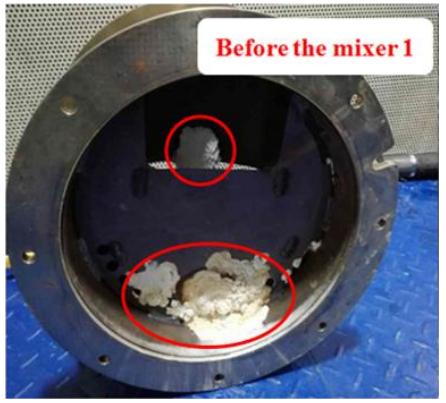
混合管段内的
液膜质量发展过程

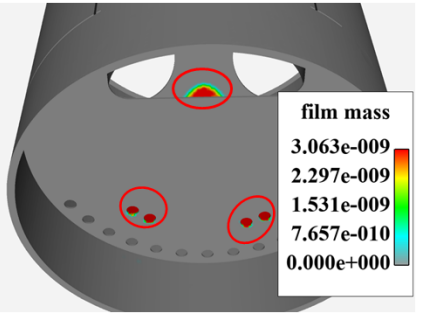


试 验

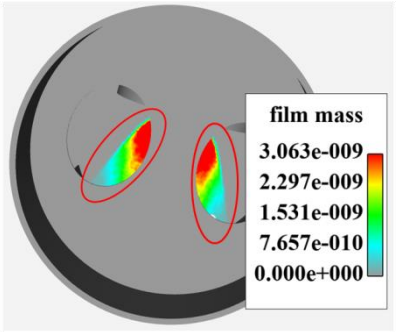
CONVERGE

混合器前





混合器后



CONVERGE

计算结果（液膜质量）与试验中沉积物位置基本一致

基于CONVERGE的数值模拟

结果分析

评价指标

➢**SCR入口的均匀性指数**

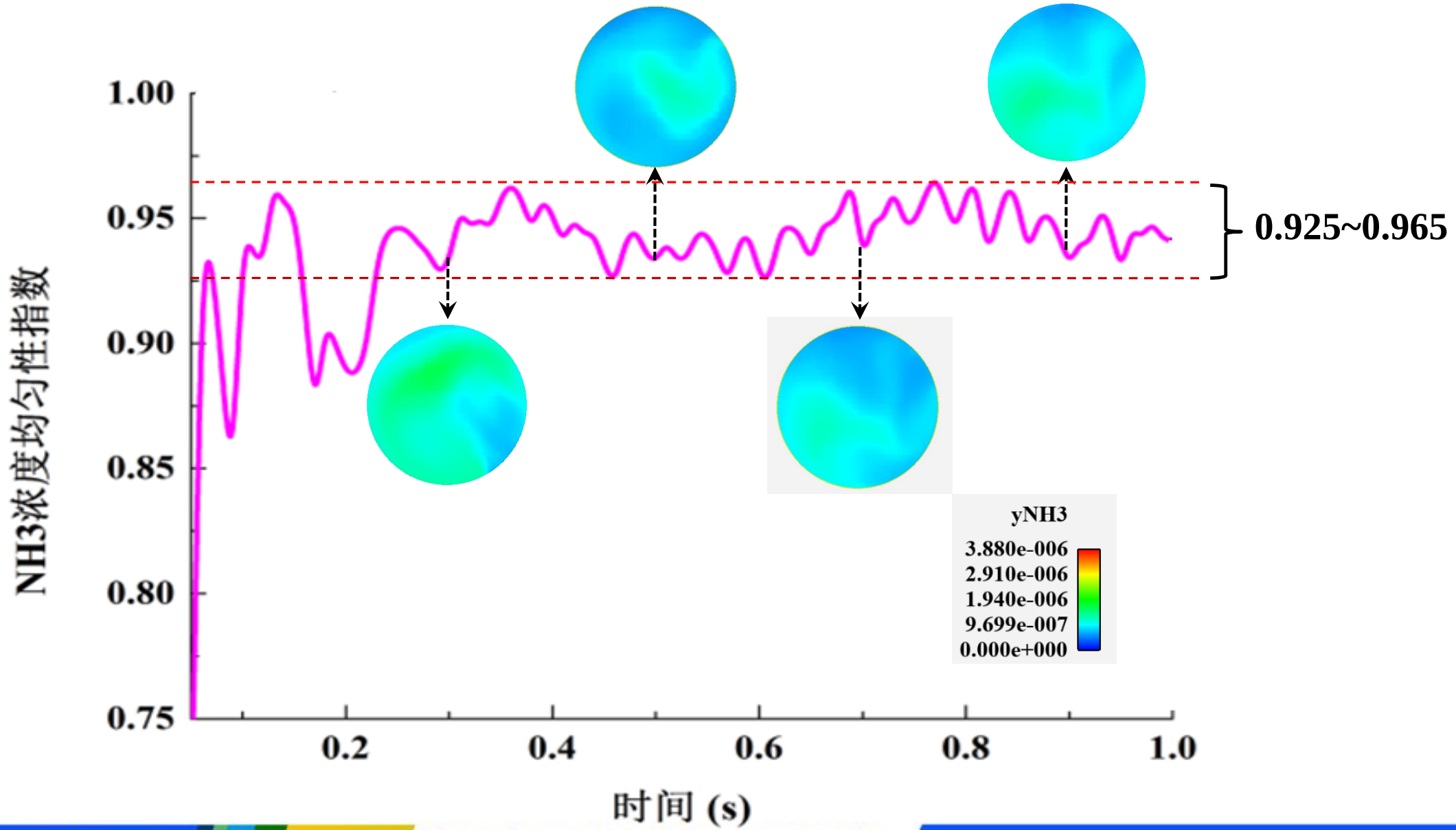
NH3浓度均匀性指数：$$U_{\mathrm{m}} = 1 - \frac{1}{2AM}\sum_{A}\sqrt{(M-m)^2}\,\Delta A$$

速度均匀性指数：$$U_{\mathrm{v}} = 1 - \frac{1}{2AV}\sum_{A}\sqrt{(V-v)^2}\,\Delta A$$

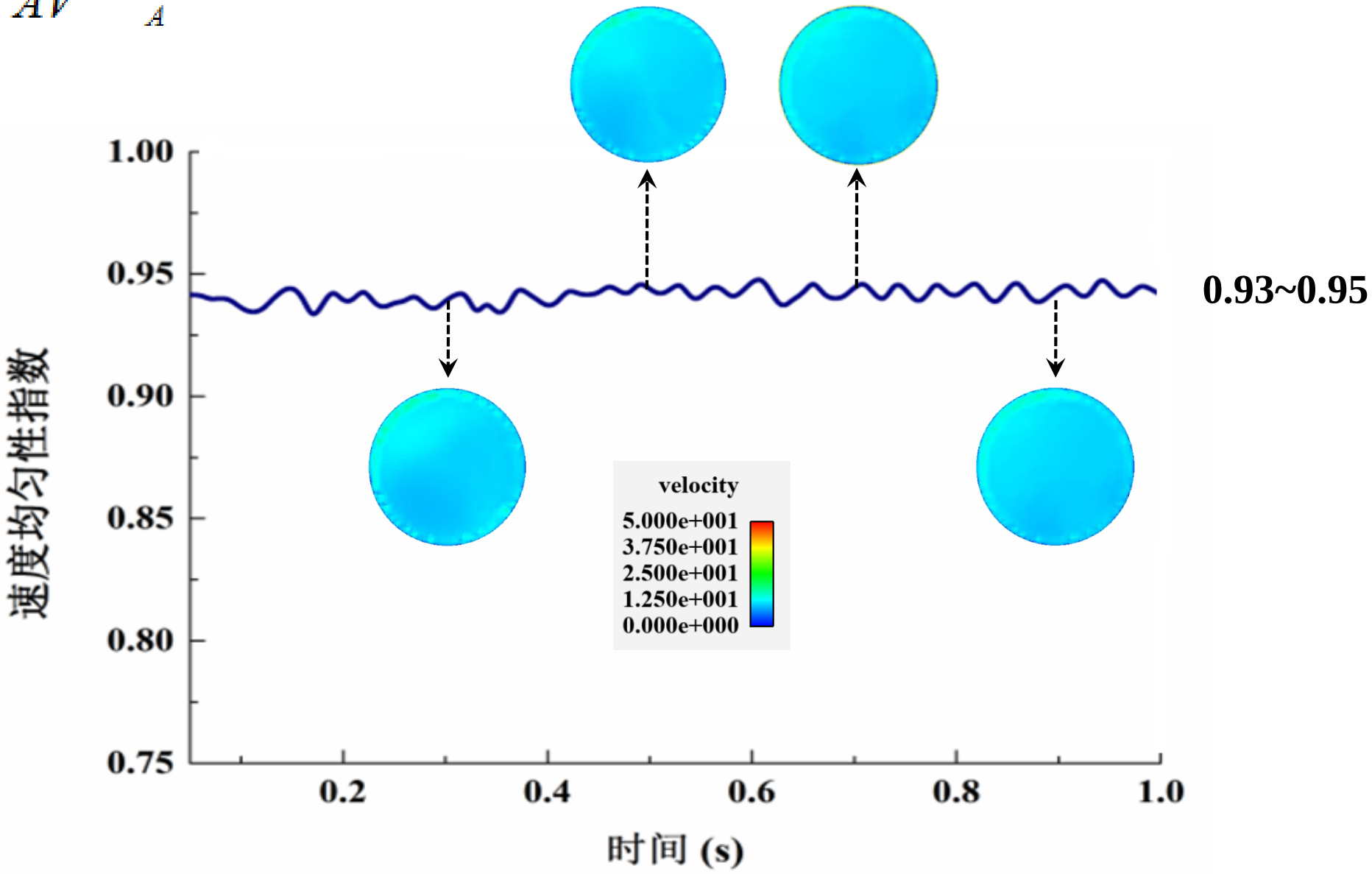
➢**混合器压差**：$$\Delta P = \frac{\sum_{i=1}^{n} P_{i,in}}{n} - \frac{\sum_{i=1}^{m} P_{i,out}}{m}$$

➢**沉积物**：成分，位置

结果分析——SCR入口的均匀性指数

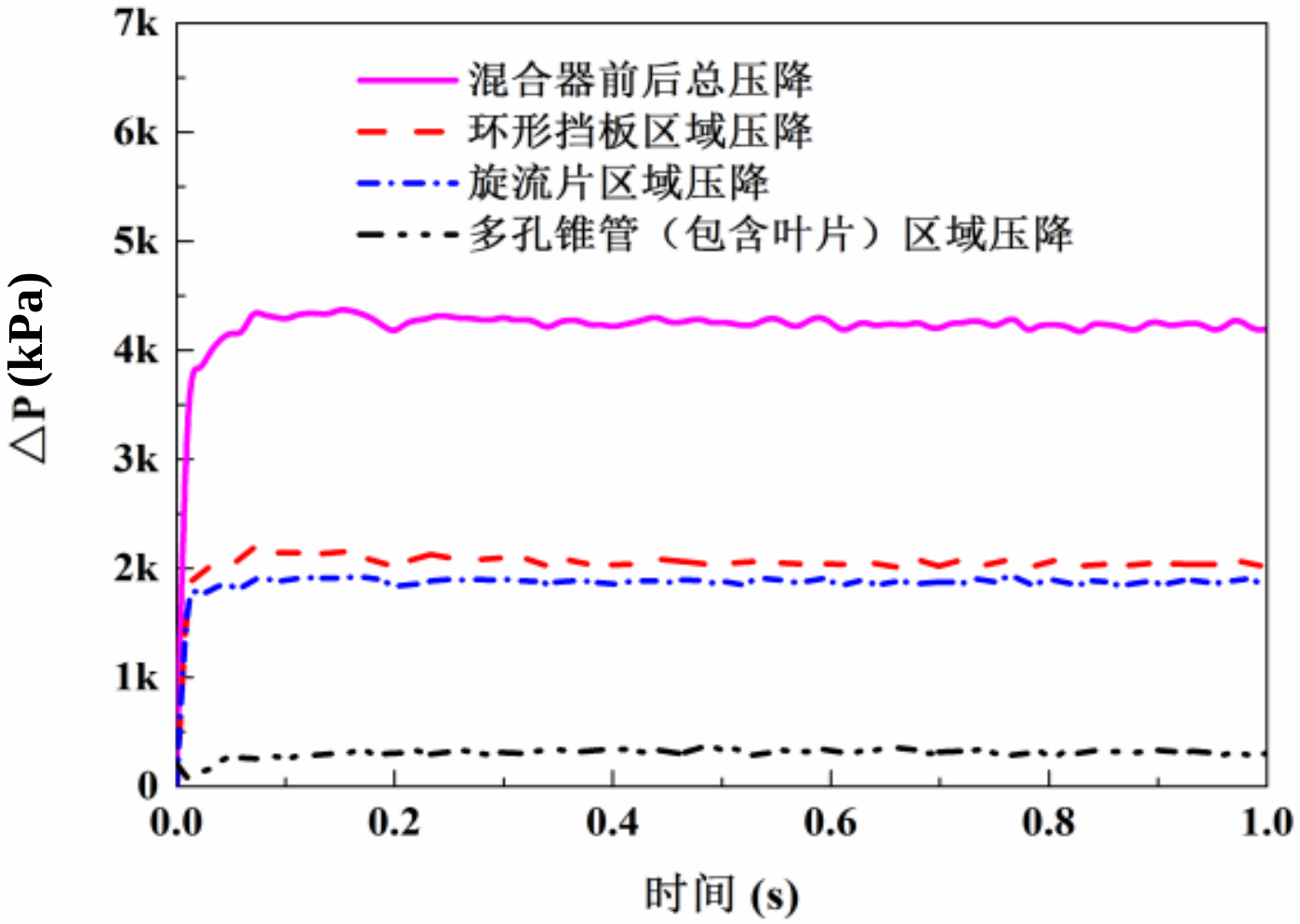


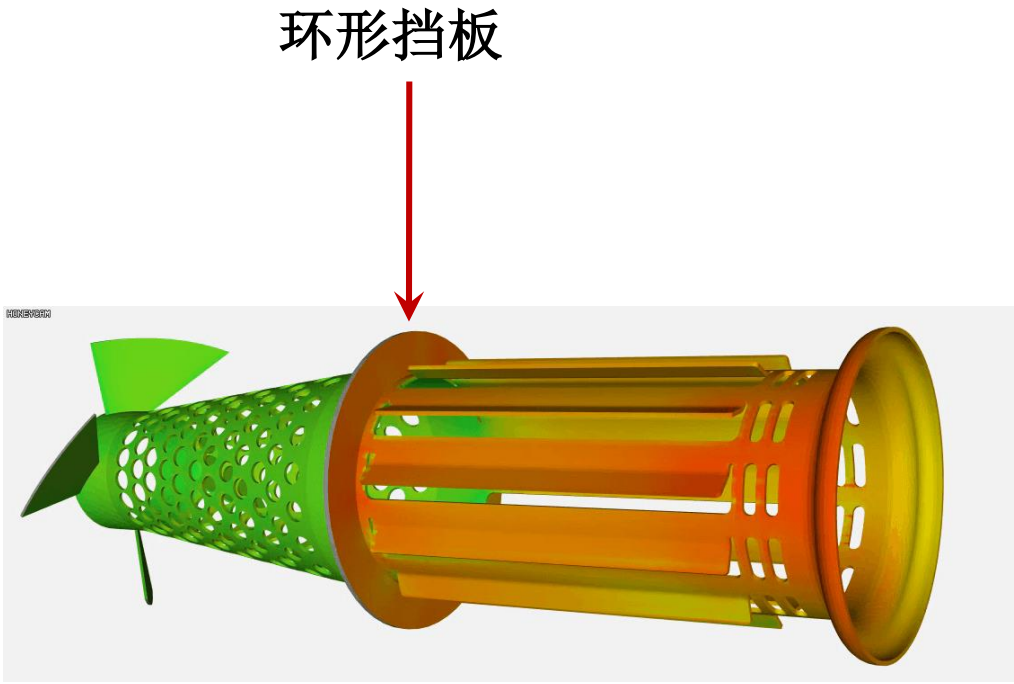
$$U_v = 1 - \frac{1}{2AV}\sum_A \sqrt{(V - v)^2}\,\Delta A$$



0.93~0.95

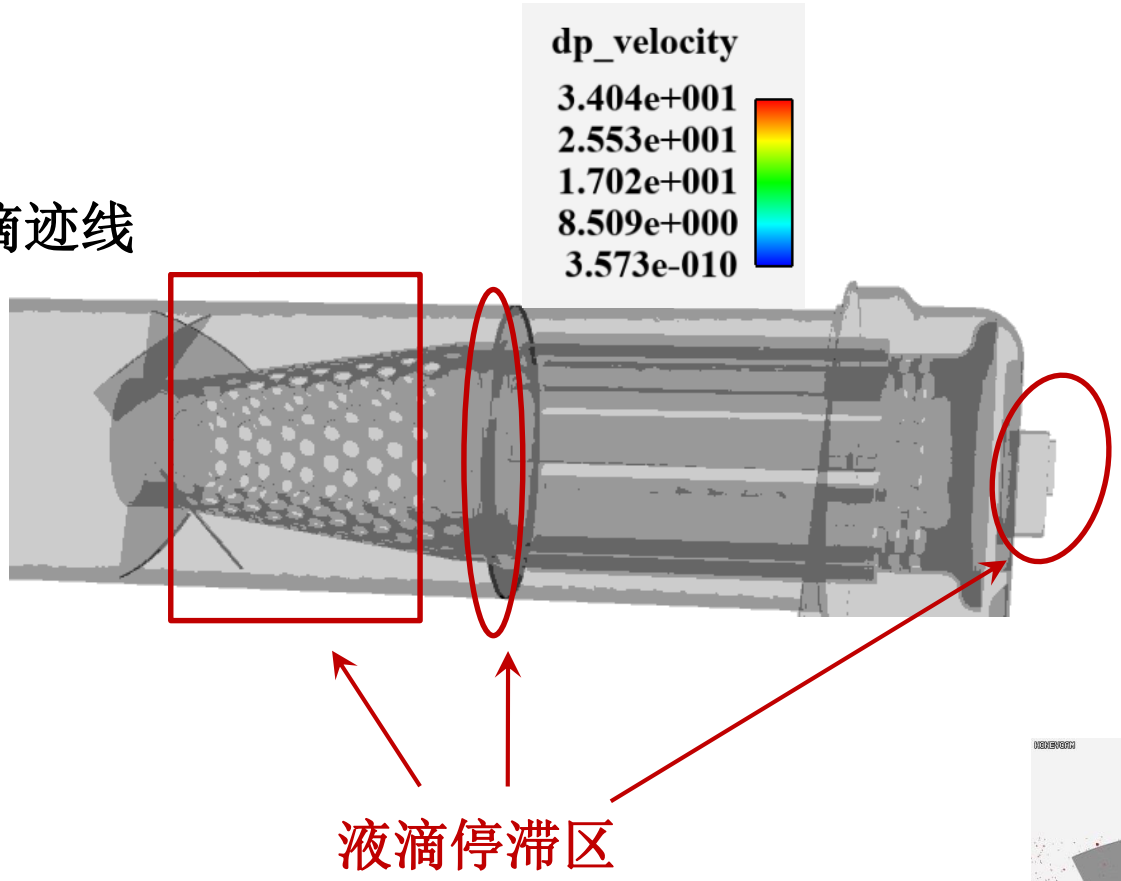
结果分析——混合器压差

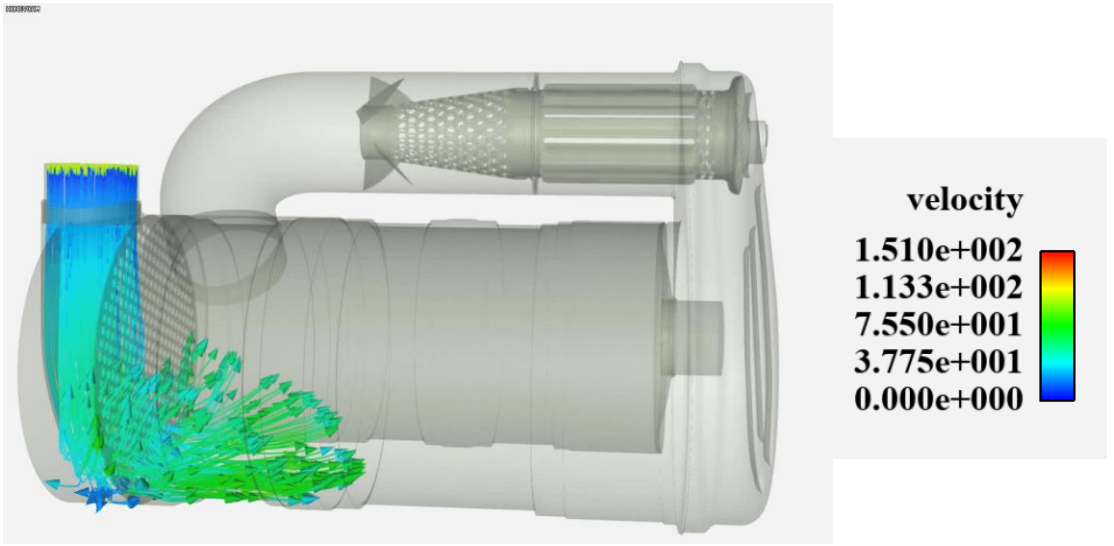


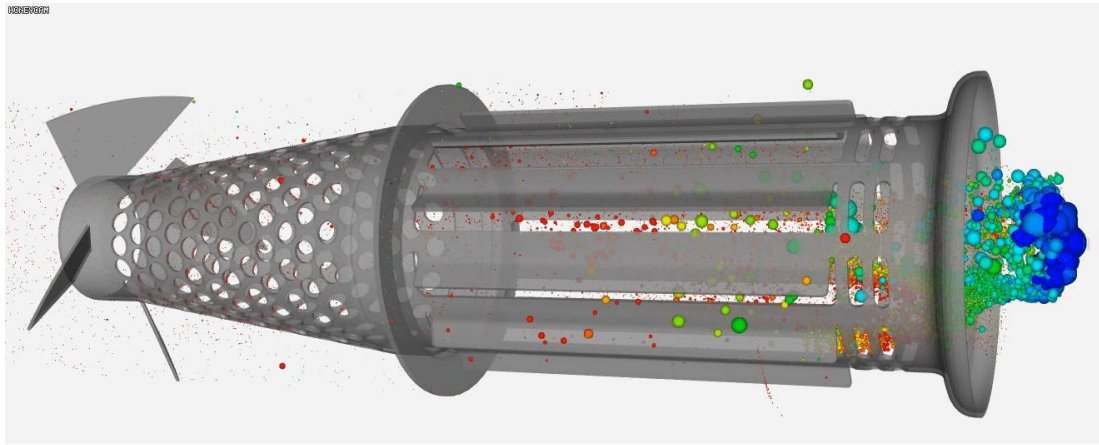


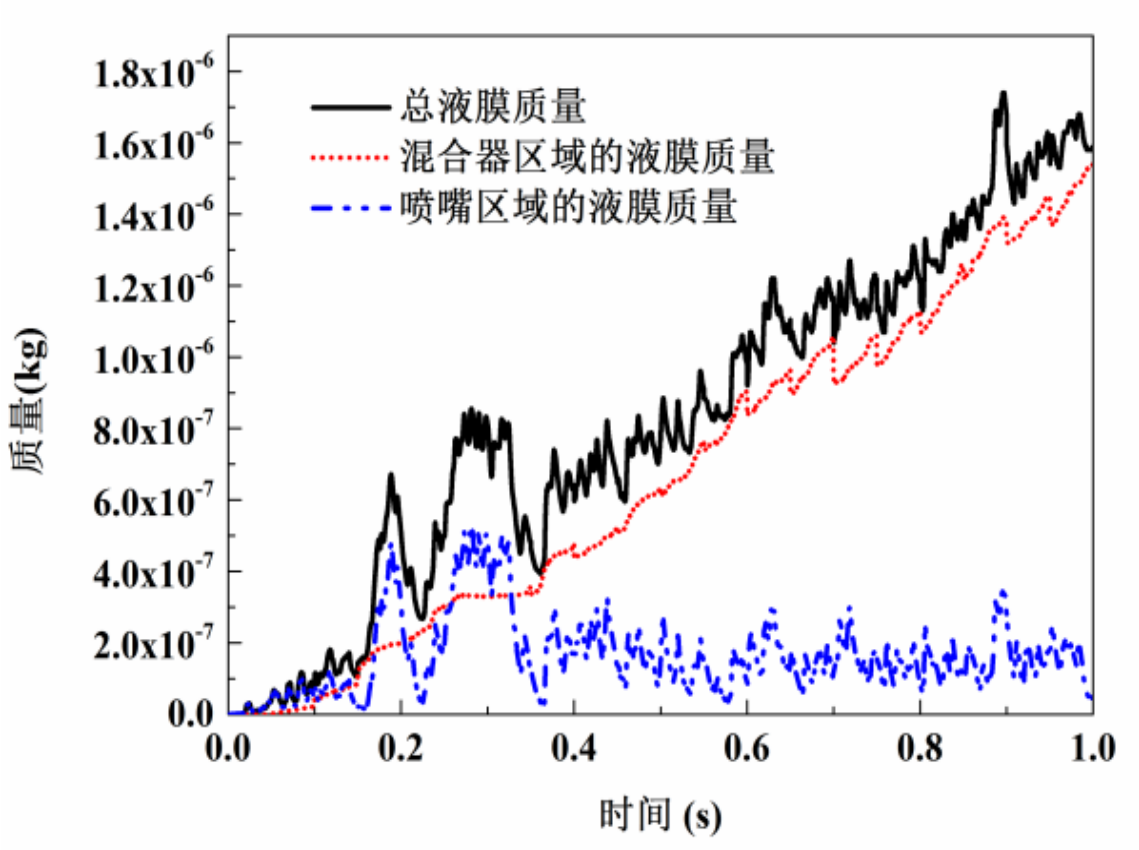
结果分析——沉积物

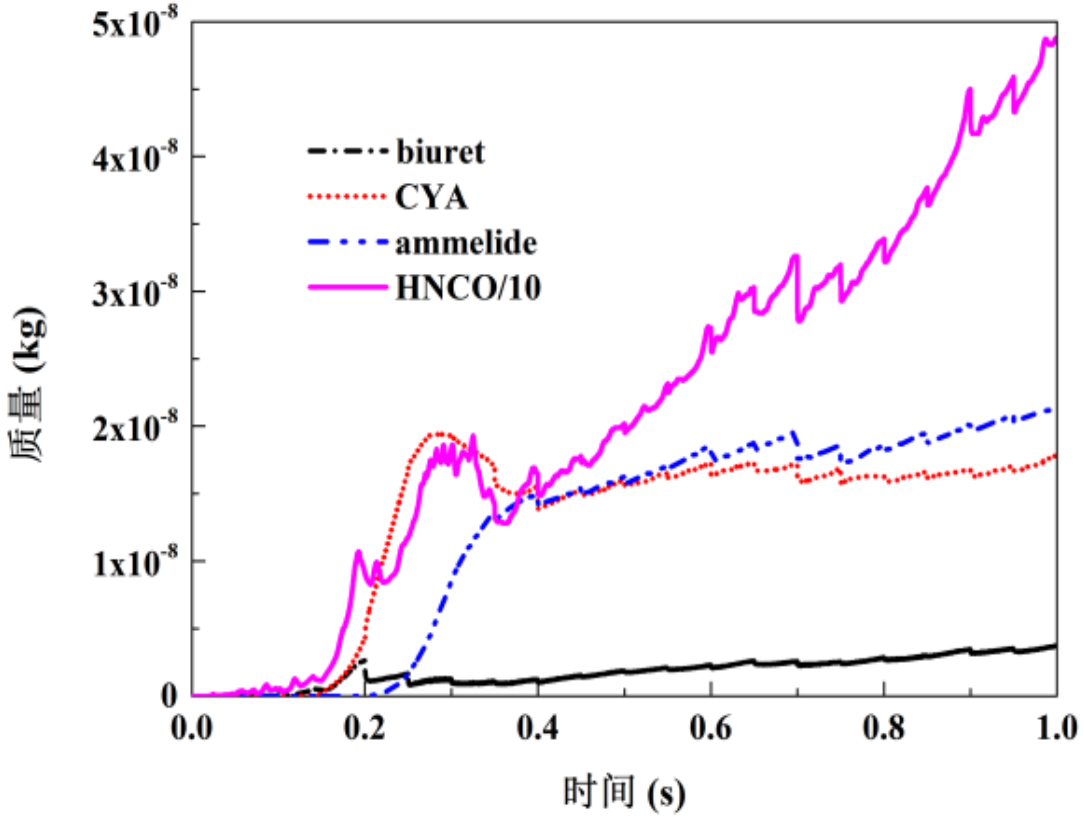
液滴迹线











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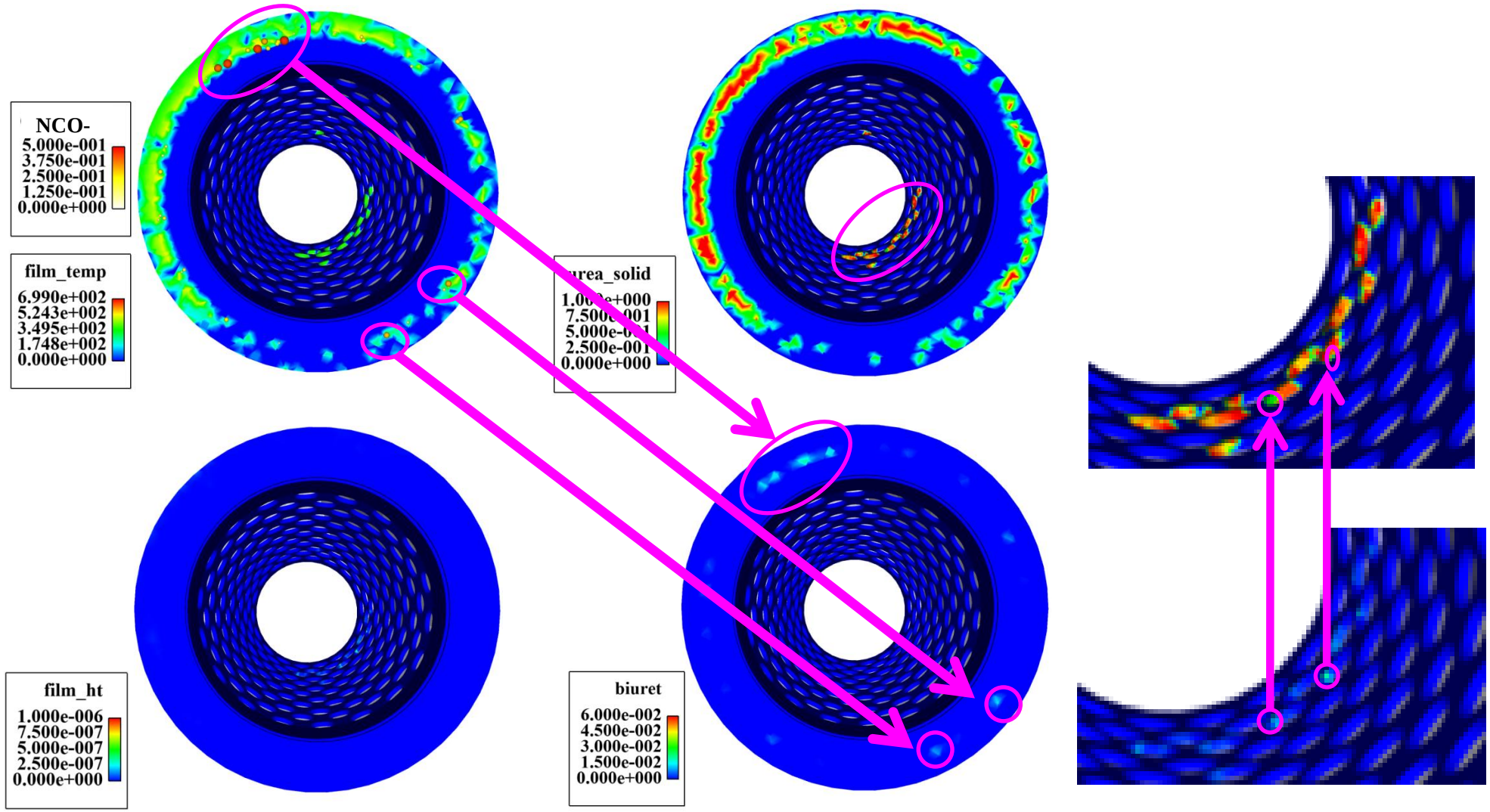

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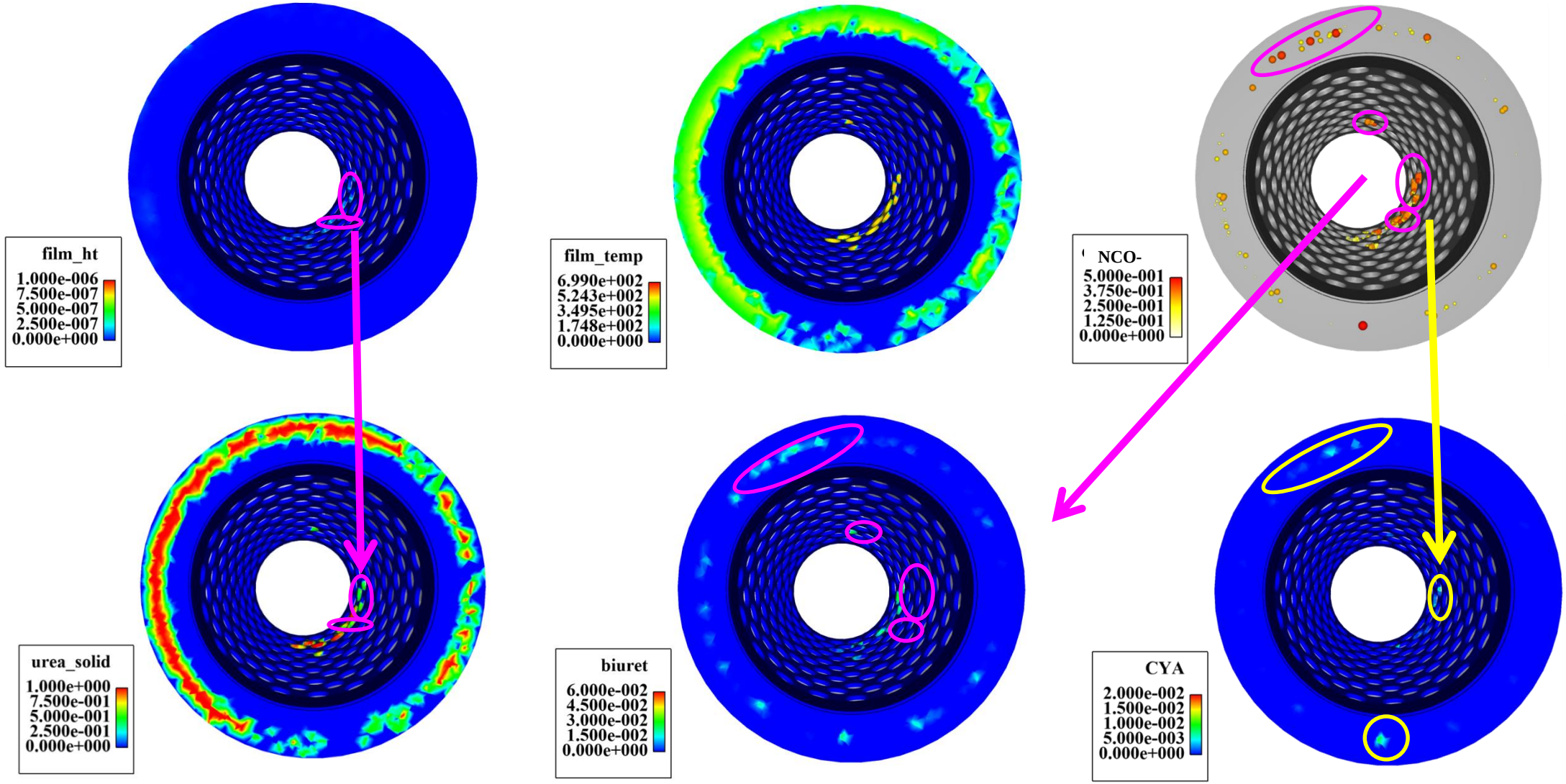

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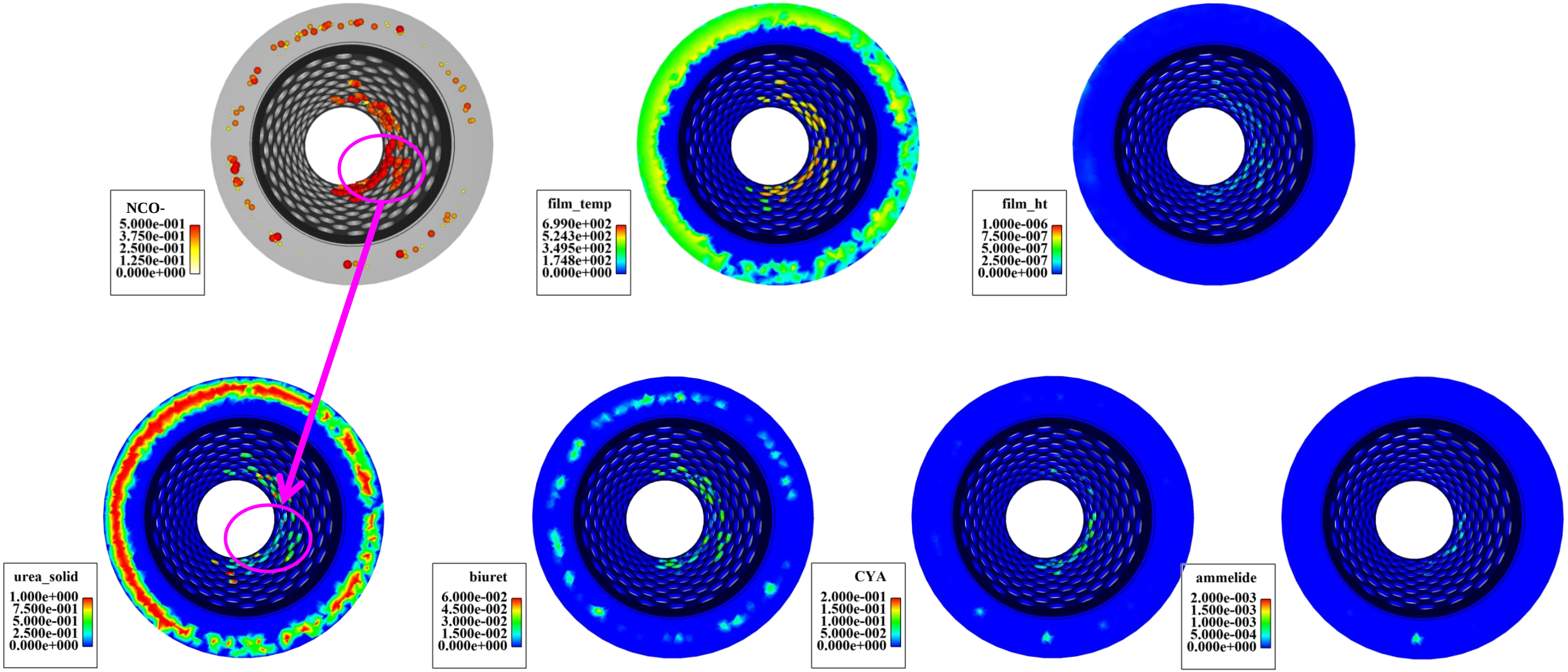
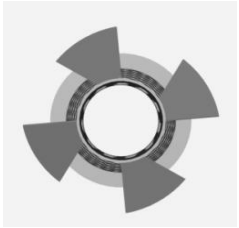
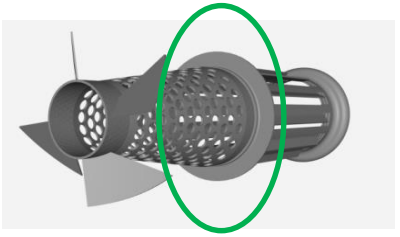
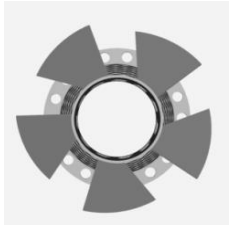
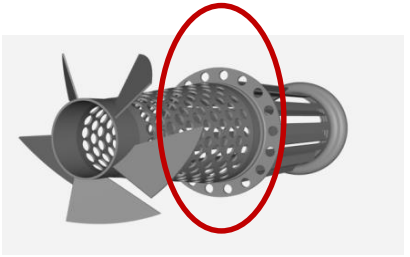
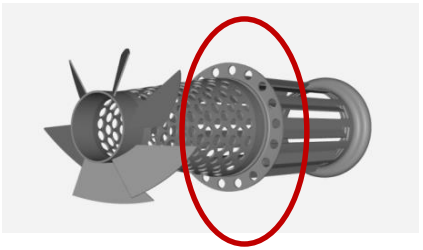
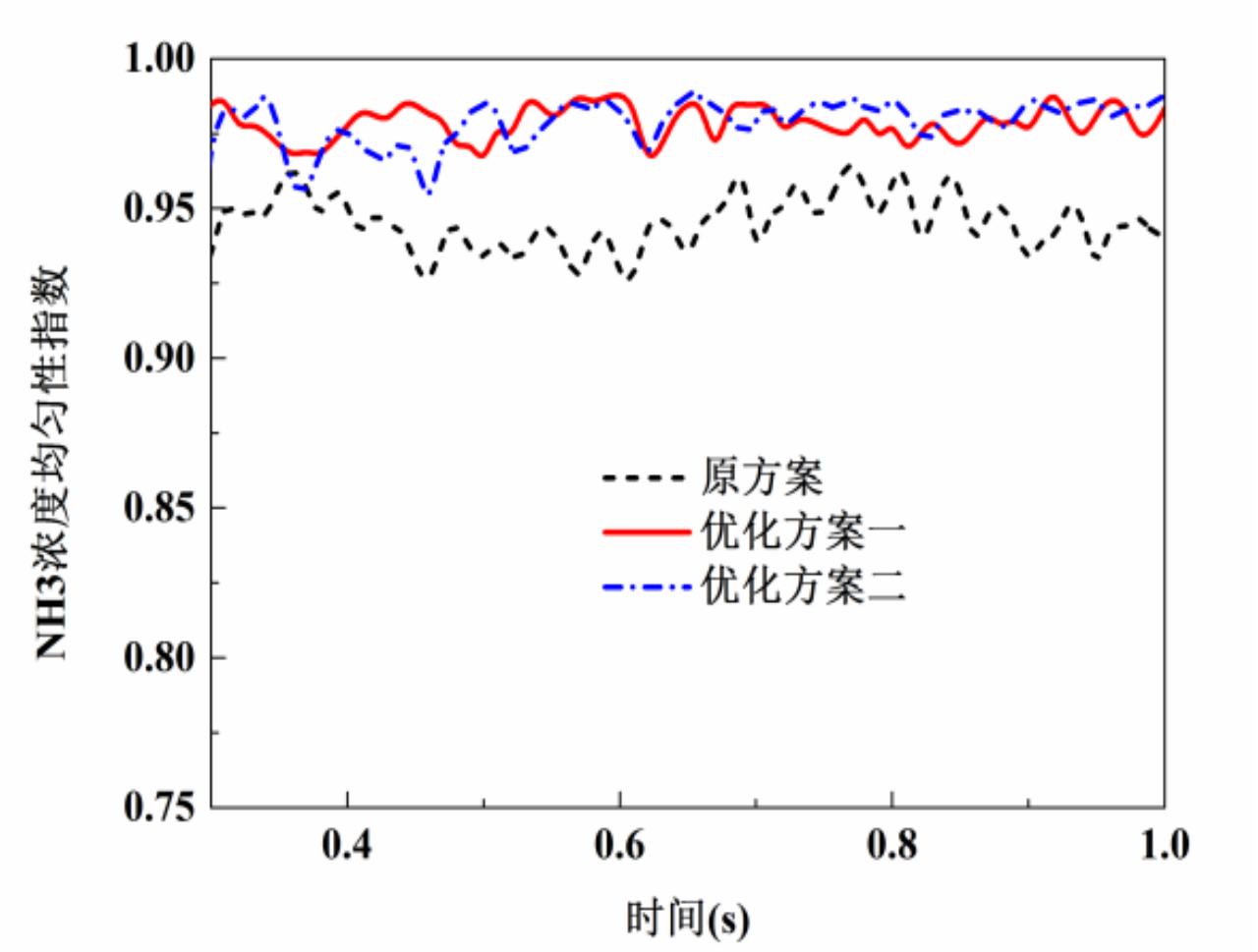


基于CONVERGE的数值模拟

混合器结构优化

原方案			4个叶片 挡板无孔
优化方案一			5个叶片 挡板均匀布置18个孔
优化方案二			6个叶片 挡板均匀布置18个孔

优化后结果分析——SCR入口均匀性指数



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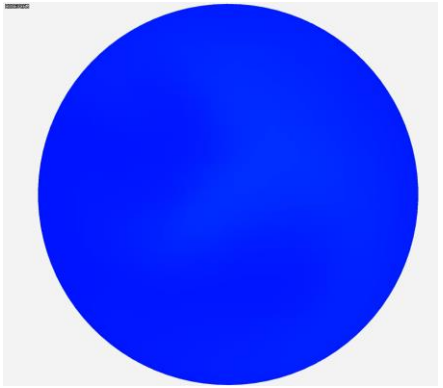
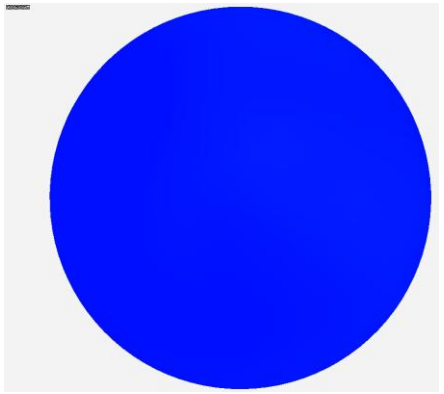


优化方案一



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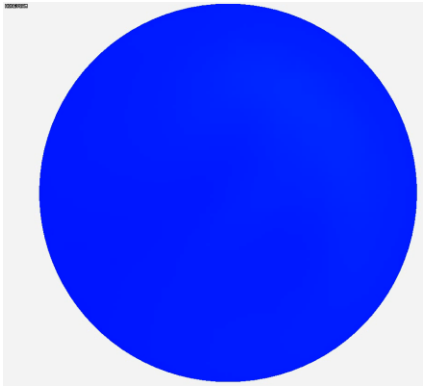

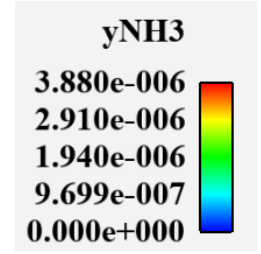

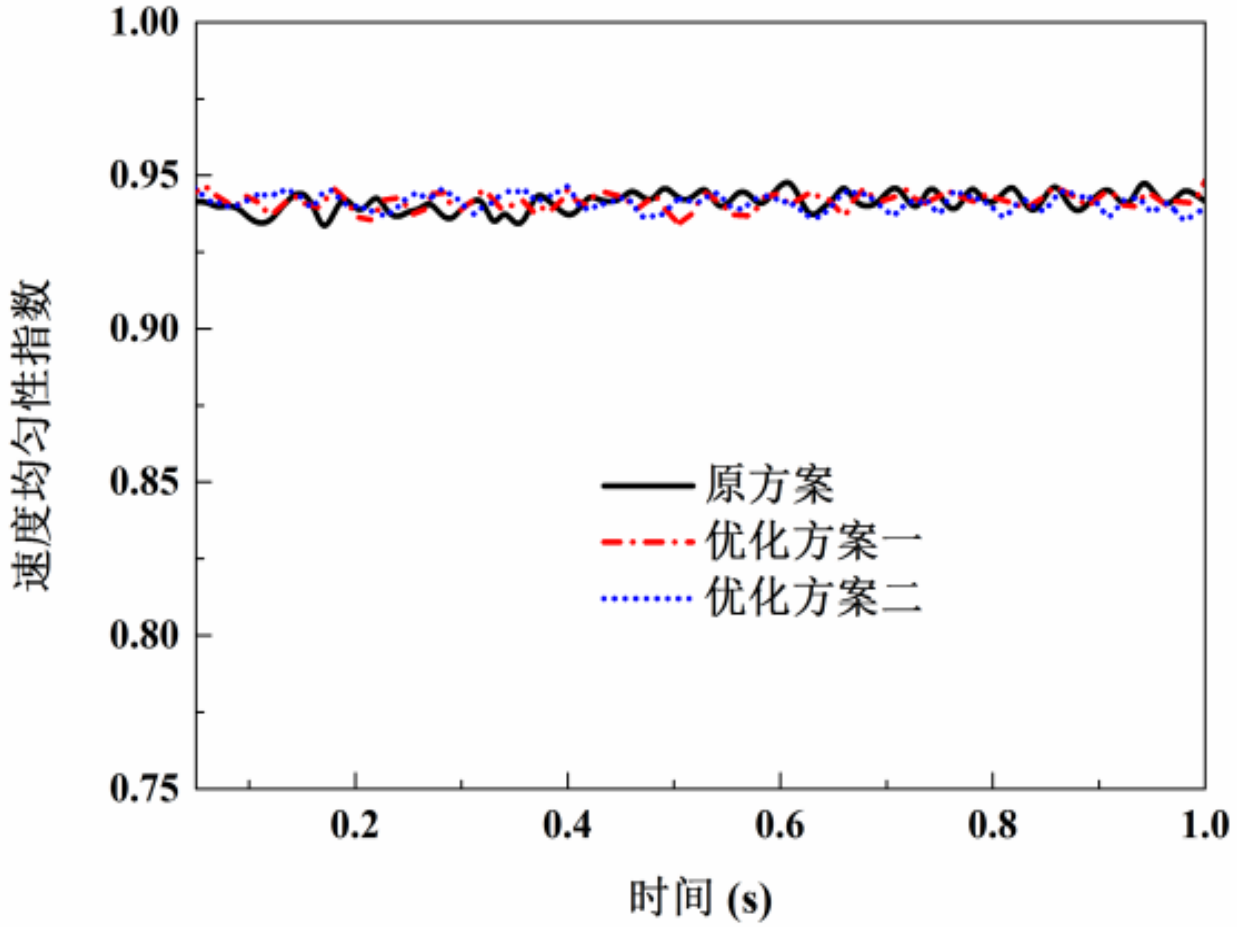

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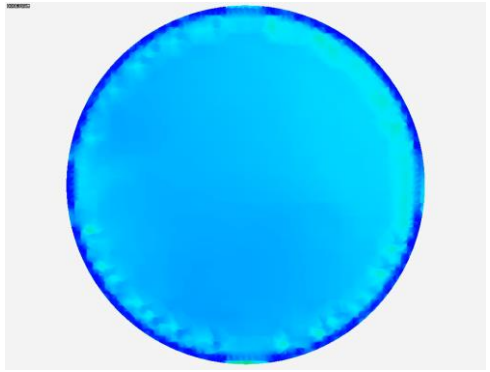
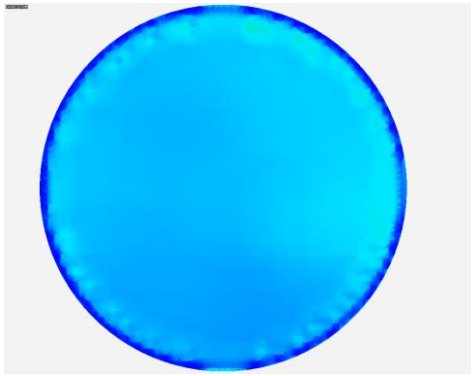
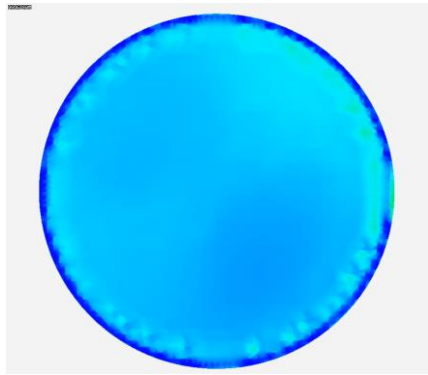
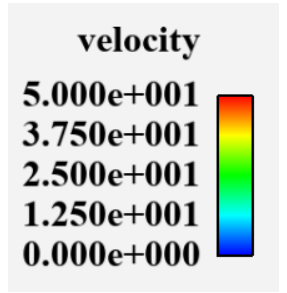


优化方案一

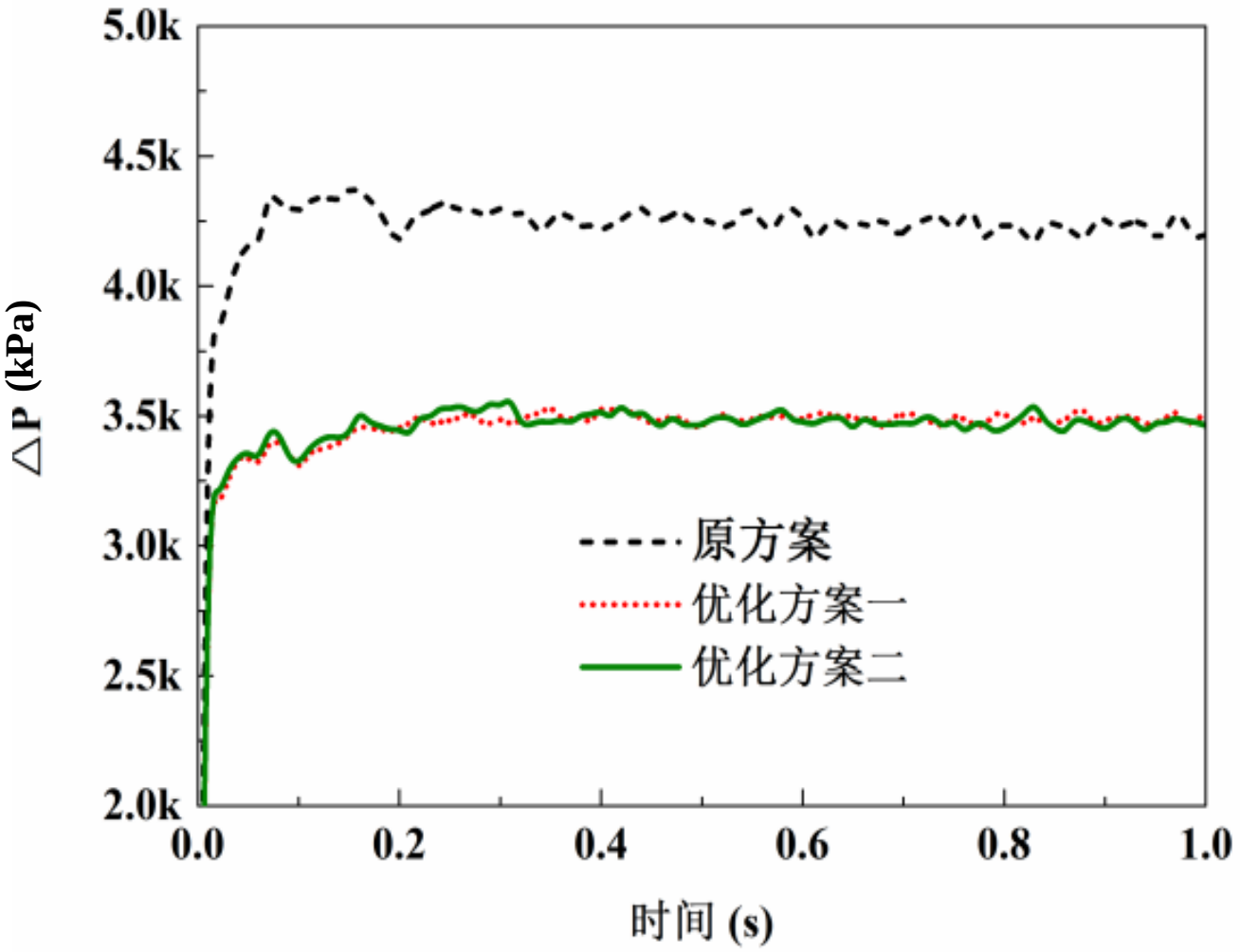


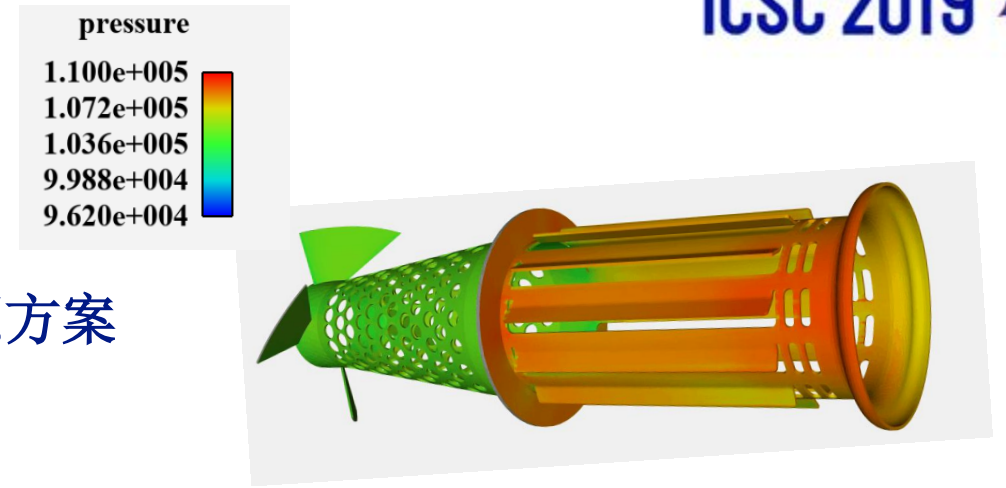
优化方案二



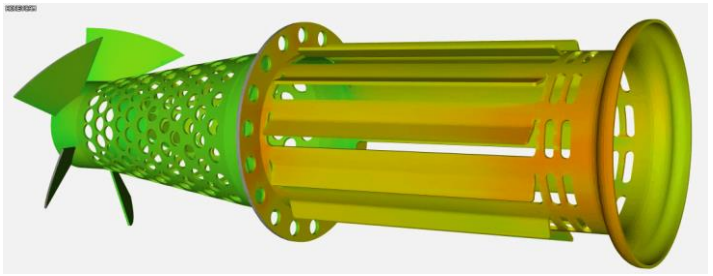


优化后结果分析——混合器压差

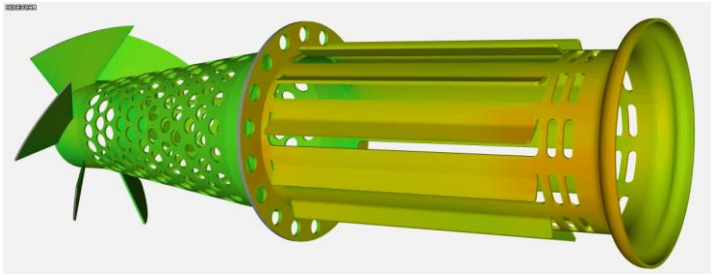




原方案



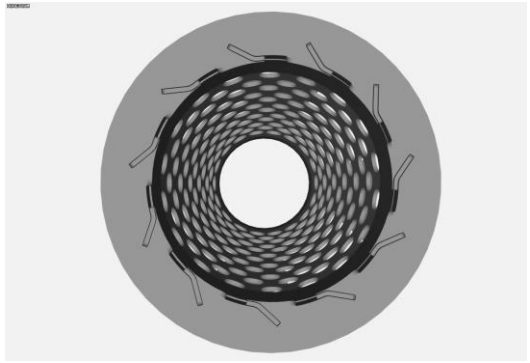
优化方案一



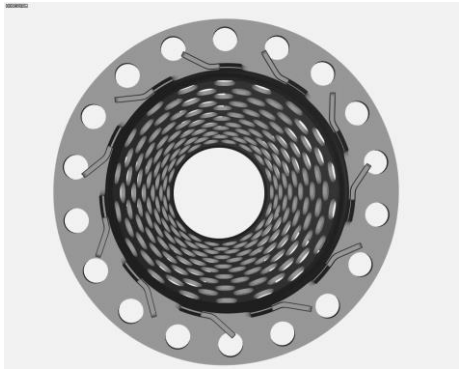
优化方案二

优化结果分析——沉积物

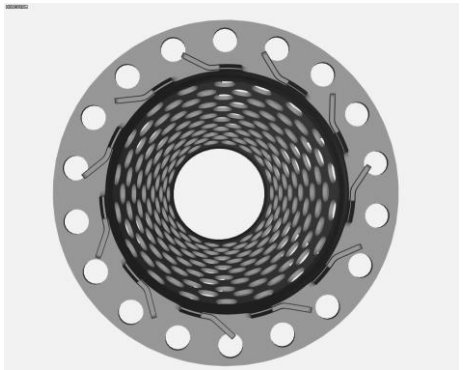
原方案

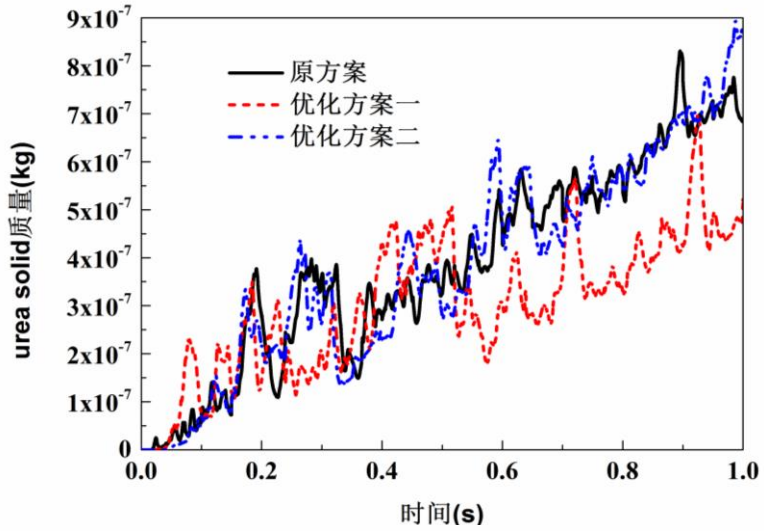


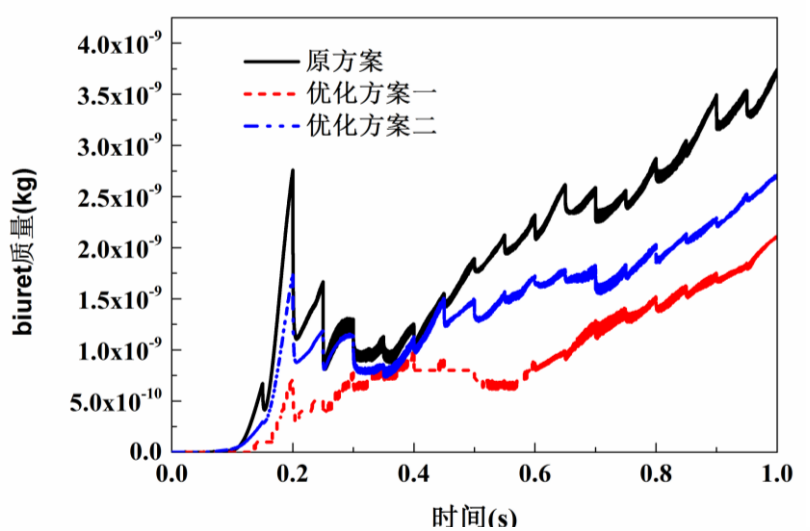
优化方案一

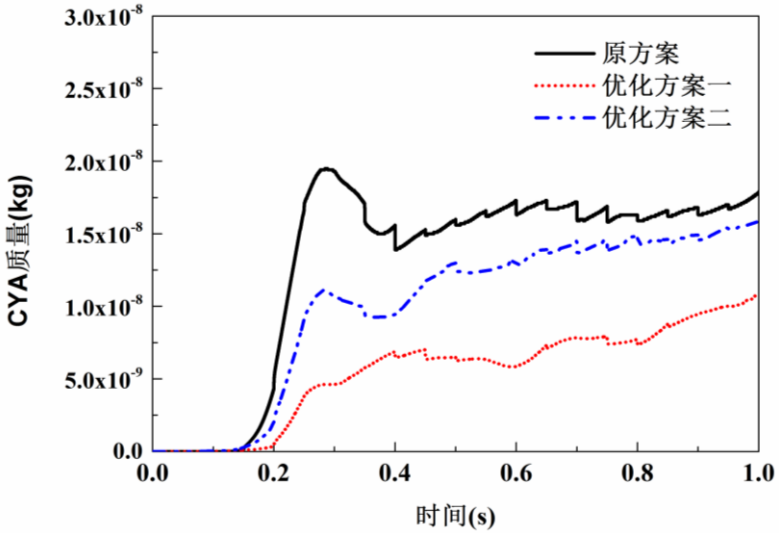


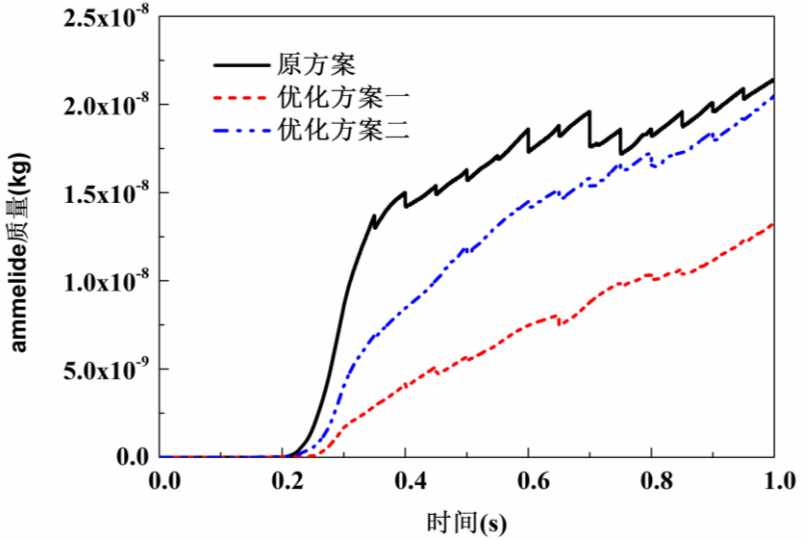
优化方案二











谢谢您的聆听