

**Perspectives From A
University Research
Administrator And Journal
Editor**

David S. Sholl
Executive Vice President for Research
Rice University



RICE UNIVERSITY

Systematic searches for replicate experiments in chemical literature provide estimates for data reliability

In 'hot' topics, multiple groups study similar materials at similar times.

Molecular adsorption in porous materials

1,065 replicates found in literature

1 in 6 experiments classified as an outlier

Park et al., *Chem. Mater.* 29 (2017) 10487

Bingel et al., *J. Chem. Eng. Data* (2022)

Synthesis of new crystalline materials

Citations of 150 materials followed for 11-17 years

Only 1 in 6 materials synthesized again

Agrawal, Han, Herath and Sholl, *PNAS* 117 (2020) 877

Sholl, *J. Phys. Chem. C* 130 (2026) 1433



Published research from research institutions is large and diverse

Rice University has annual R&D expenditures of ~\$250M

Many large US universities (especially with medical schools) have annual R&D expenditures > \$1B

Rice University faculty published ~73,000 papers from 2005-2025

~10 papers/day

DOE National Labs require internal review before paper submission

This idea would be viewed in horror by university faculty

Quality of internal review is highly variable (similar to external peer review)



Journals can take steps to increase data transparency



- Relatively large journal (~1000 submissions each year)
- Generalist journal covering all topics in field (process systems, thermodynamics, catalysis, separations, particle technology, bioengineering, ...)
- 1 Editorial Assistant and Editor-in-Chief see all submissions; peer review handled by 9 Associate Editors
- >80% of submissions are from China



“Data is available upon request...” is not a solution

Prior to 2023, AIChE Journal authors required to include statement similar to
“Data supporting this study is available from the authors upon reasonable request”

Does this work?

This question has been empirically tested in the psychological literature

Wicherts, J. M. et al., The poor availability of psychological research data for reanalysis, Am. Psychol., 2006, 61, 726-8;
Hussey, I., Data is not available, PsyArXiv preprint, 2023, <https://psyarxiv.com/jbu9r>

< 20% of authors shared data when requested (for papers published in last 5 years)



Checking a past issue of AIChE Journal showed challenges with accessing data

All papers in September 2022 issue examined, asking “Can numerical data underlying the paper’s figures be easily accessed?”

Only 1 paper tabulated the study’s data in SI

18% of papers had no SI

SI varied strongly in length and format

1 paper used a GitHub repository in addition to SI



AIChE Journal implemented new data sharing standards in 2023

Read full details at [10.1002/aic.18017](https://doi.org/10.1002/aic.18017)

Element 1: All submissions are *required* to include SI that at a minimum includes tabulated numerical data for “all” figures in the manuscript

Element 2: All submissions must include a section titled “*Data Availability and Reproducibility*” that lists where data for Figures is available and discusses how error bars were defined, experiments/calculations were validated etc.

Submissions without both of these required elements are rejected without review (but allowed to resubmit)

Bottom line: this change has caused minimal disruption for the journal



Examples from post-2023 papers in AIChE Journal

3.4 | Data availability and reproducibility statement

The numerical data from Figures 1, 2, 7, 8, 10–12 are available as a .zip file in [Supporting Information](#), this .zip file includes a compilation of input files that are described in Figures 1, 2, 7, 8, 10–12.

Liu et al.
10.1002/aic.18201

3.5 | Data availability and reproducibility statement

The numerical data from Figures 1, 2, 5B, and 7A,B are tabulated in the [Supporting Information](#). The highly efficient 0.1Ni/Mo_xN catalyst was selected to confirm there was no external and internal diffusion limitations under the adopted condition (see in [Supporting Information](#)). The equipment used for ammonia synthesis test had been validated with good reliability in our previous report.²⁰

Li et al.
10.1002/aic.18194



AIChE Journal's approach suggests proactive actions by individuals and departments

As a Journal Editor/Advisory Board member...

Advocate that your journal adopt the AIChE Journal model (or a better one)

I would be happy to talk with your Editor-in-Chief

Key resource: *10.1002/aic.18017*

As a reviewer...

Include a standard request for data sharing in every review

An example from the Center for Open Science:

"I request that the authors add a statement to the paper confirming whether, for all experiments, they have reported all measures, conditions, data exclusions, and how they determined their sample sizes. The authors should, of course, add any additional text to ensure the statement is accurate. This is the standard reviewer disclosure request endorsed by the Center for Open Science [see <http://osf.io/hadz3>]. I include it in every review."

As a researcher...

Adopt standardized data sharing policies in your group

Ask students about reproducibility in thesis proposals/defenses etc.

Key resource: *10.1021/acs.langmuir.9b02963*

