Stochastic pix2vid: A new spatiotemporal deep learning method for image-to-video synthesis in geologic CO_2 storage prediction

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Abstract

Numerical simulation of multiphase flow in porous media is an important step in understanding the dynamic behavior of geologic CO_2 storage (GCS). Scaling up GCS requires fast and accurate high-resolution modeling of the storage reservoir pressure and saturation plume migration; however, such modeling is challenging due to the high computational costs of traditional physics-based simulations. Deep learning models trained with numerical simulation data can provide a fast and reliable alternative to expensive physics-based numerical simulations. We present a Stochastic pix2vid neural network architecture for solving multiphase fluid flow problems with superior speed, accuracy, and efficiency. The Stochastic pix2vid model is designed based on the principles of computer vision and video synthesis and is able to generate dynamic spatiotemporal predictions of fluid flow from static reservoir models, closely mimicking the performance of traditional numerical simulation. We apply the Stochastic pix2vid model to a highly-complex CO_2-water multiphase problem with a wide range of reservoir models in terms of porosity and permeability heterogeneity, facies distribution, and injection configurations. The Stochastic pix2vid method is first-of-its-kind in static-to-dynamic prediction of reservoir behavior, where a single static input is mapped to its dynamic response. The Stochastic pix2vid method provides superior performance in highly heterogeneous geologic formations and complex estimation such as CO_2 saturation and pressure buildup plume determination. The trained model can serve as a general-purpose, static-to-dynamic (image-to-video) alternative to traditional numerical reservoir simulation of 2D CO_2 injection problems with up to 6,500× speedup compared to traditional numerical simulation.

Keywords: Image-to-video synthesis, Spatiotemporal prediction, Convolutional neural network, Recurrent neural network, Proxy model

1 Introduction

Geologic CO_2 sequestration (GCS) has emerged as a potential technology solution to reduce anthropogenic greenhouse gas emissions to the atmosphere [1–3], and has become increasingly popular worldwide due to the need to meet international climate protection agreements [4–6]. Modeling injected CO_2 movement in the subsurface over and beyond the life of the project is a critical component to support optimum GCS project decision making for safe and secure CO_2 sequestration. A schematic of typical GCS operations is shown in Figure 1, including storage in depleted oil and gas reservoir and deep saline formations, and CO_2 enhanced oil and coalbed methane recovery [7–9]. However, there are several technical challenges associated with the subsurface models to support GCS operations. In order to accurately forecast and monitor subsurface multiphase flow, physics-based high-fidelity numerical simulations are required. These numerical simulations are computationally intensive and time-consuming since they require iterative solutions of nonlinear systems of equations applied over large volumes of the subsurface at sufficient resolution to represent heterogeneity [10–12]. Also, due to the large degree of uncertainty in subsurface data, and the spatial distribution of the properties of heterogeneous porous media between the sparsely sampled data, GCS operations require a robust probabilistic-based uncertainty assessment for improved engineering decision-making [13–15]. In order to capture the fine-scale multiphase flow behavior given an uncertain spatial distribution of subsurface properties, a large number of numerical simulations are required, leading to very high computational costs [16, 17].

To overcome this, machine learning techniques have emerged as candidate proxy models due to their ability to perform dimensionality reduction for efficient problem parameterization, and to calculate fast predictions of subsurface flow and transport behavior for real-time feedback on the impact of geological and engineering controls on CO_2 behavior in the subsurface over time [18–20]. Dimensionality reduction techniques are supervised or unsupervised machine learning methods that compress (or encode) the data, X, into a lower-dimensional latent feature representation, z, and decompress (or decode) the latent representation either: (1) back to the original data space, $\hat{X}$ (unsupervised, AutoEncoder), or (2) to a new target feature space, y (supervised, Encoder-Decoder) [21, 22], as shown in Figure 2. These are enabled by recent advancements in deep learning algorithms and in computing architecture and power, enabling GPU-enabled neural network models that have accelerated the fields of forward and inverse modeling [23, 24]. Classical statistical modeling methods are often hindered by the size of the models and their conditioning to big data, i.e., that is data with volume, velocity, variety, value, and veracity [25, 26]. By analyzing big data sets, machine learning techniques can uncover complex patterns and relationships in lower-dimensional, latent feature representations that may not be discernible through traditional statistical and geostatistical methods [27–29].

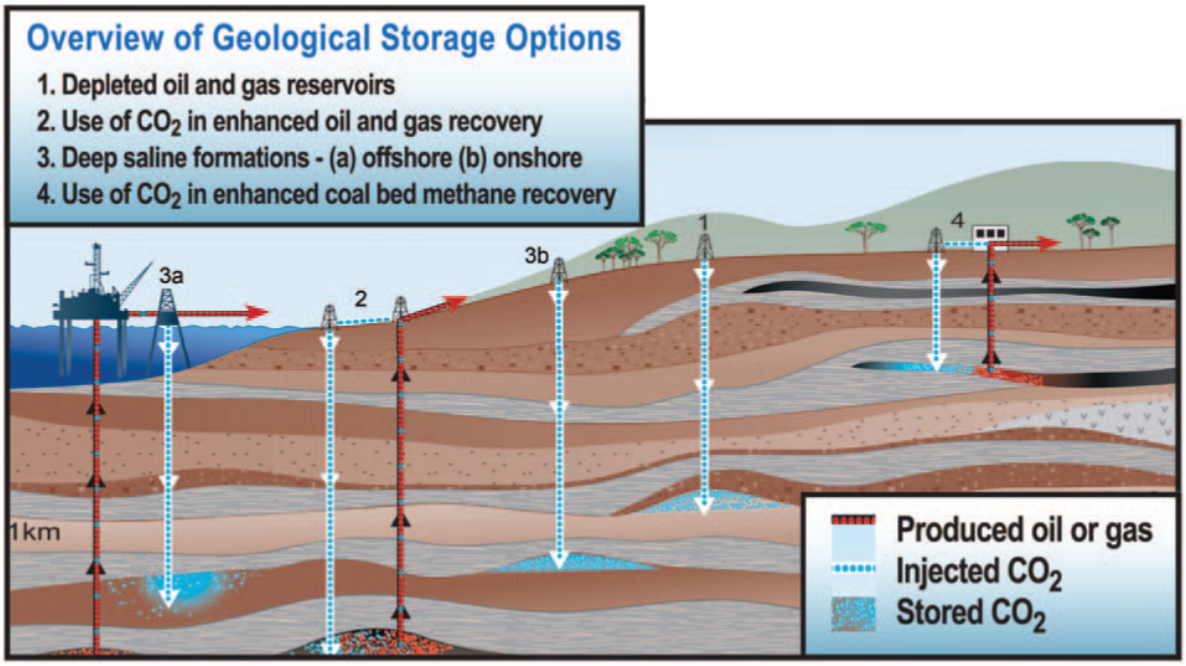

Figure 1: Types of geologic CO_2 storage operations and the geologic formations that can be used for sequestration. *Modified from the Carbon Dioxide Cooperative Research Center (CO2CRC), http://www.co2crc.com.au/about/co2crc*

When combined with a latent space modeling framework, machine learning approaches can efficiently and accurately exploit hidden features in the data, removing redundancies or noise, and decreasing the order of the problem significantly [30, 31].

Machine learning approaches applied to the subsurface are divided into two main categories, namely purely data-driven models or physics-informed models. Data-driven proxy models, or data mapping operators, are neural network architectures trained with labeled data that produce a mapping from input predictor features to output response features [32, 33]. On the other hand, the training process to match

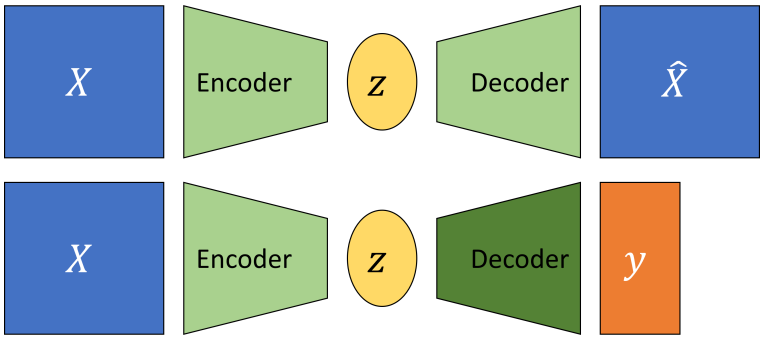

Figure 2: Dimensionality reduction model structure. Unsupervised AutoEncoder structure (top), and supervised Encoder-Decoder structure (bottom).

training data for PINNs is regularized with the minimization of the (physical) loss from the residual of the governing partial differential equations (PDEs) along with the losses associated with the initial and boundary conditions [34, 35]. However, other variants of PINNs such as physics-guided or physics-constrained neural networks - where the PDE loss is not embedded in the training but the models have specific architectures or parameters to mimic the physics in the system - have proven useful for subsurface energy resource engineering applications [36–38]. One disadvantage of machine learning techniques is that they require significant amounts of training data but once trained, these prediction models can be applied over a wide variety of settings and conditions for which they have been specifically trained [39, 40], but suffer from lack of generalization, i.e., inability to provide accurate predictions away from the training data. For both data-driven and physics-informed approaches, typically, spatial relationships are modeled through convolutional neural networks (CNNs) [41, 42] and the temporal relationships through recurrent neural networks (RNNs) [43, 44], but recent advancements in transformer-based architectures improve performance compared to the CNN and RNN methods for spatial and temporal latent feature representations [45–47]. In general, efficient compression of the input features into a representative latent space is proven as an effective approach for spatial and temporal parameterization of the forward or inverse problem.

A number of machine learning-based proxy (or surrogate) models have been developed to estimate the reservoir behavior in subsurface energy resource applications. Most techniques rely on the concept of image translation, or pix2pix, where a target image(s) is predicted from an input image(s) [48–51], as shown in Figure 3. Maldonado-Cruz and Pyrcz [52] develop a convolutional U-Net model to predict pressure and saturation states given an uncertain geologic realization. This work is an example of image-to-image static forecasting, where the time state is given as an input, and the proxy model will predict a single response state of pressure and saturation at the given time. Wen et al. [53] develop a Fourier Neural Operator (FNO) architecture to predict image-to-image response states of pressure and saturation from an uncertain geologic realization and was further extended for multi-scale and nested domains [54]. These methods are based on a pix2pix, or image-to-image prediction, where a specific timestep is used as an input feature to predict the relationship between the geologic model and the reservoir response at that specific timestep. This implies that pix2pix or image-to-image methods are formulated as an even-determined or sometimes over-determined estimation problem, where the number of input features is equal to or greater than the number of output features. Moreover, numerous other proxy models have been developed for subsurface applications using more complex architectures such as generative adversarial networks (GANs) [55] and transformers [56, 57]. Despite showing consistent results and significant speedups compared to traditional numerical simulation, pix2pix models do not capture the spatiotemporal relationships and dynamic response of the subsurface system.

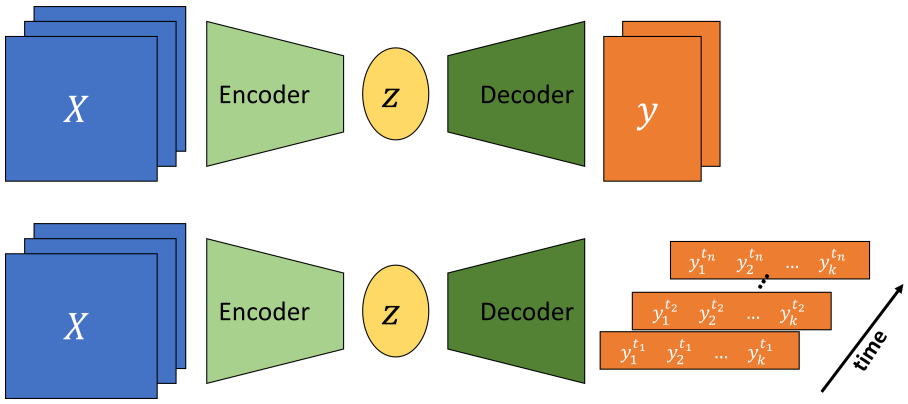

Figure 3: Image-to-image (pix2pix) (top) and image-to-timeseries Encoder-Decoder (bottom) structures.

Moving beyond image-to-image predictions, Kim and Durlofsky [58] develop a convolutional-recurrent proxy for pix2time, or image-to-timeseries, forecasting and discuss its advantages for closed-loop reservoir management under geologic uncertainty. This method moves beyond the image-to-image forecasting and exploits a spatiotemporal latent space in an encoder-recurrent neural network architecture to obtain well flow rates and pressures over time from a static geologic realization. The image-to-series formulation can still be an even- or over-determined estimation problem, where we have equal or more inputs than outputs, as shown in Figure 3. Furthermore, Tang et al. [59, 60] and Jiang and Durlofsky [17] develop a recurrent residual U-net (R-U-net) proxy for the prediction of dynamic pressure- and saturation-over-time from uncertain geologic realizations using an encoder-recurrent-decoder architecture. These methods aim to obtain dynamic response states over time from a single static input. This type of proxy model is formulated to resolve the more complex under-determined estimation problem (compared to even- or over-determined), where the number of input features is a fraction of the number of output features. However, the recurrent R-U-net proxy is limited by the fact that only the latent space receives spatiotemporal processing, while the model reconstruction is done via time-distributed deconvolutions, treating time as an additional "spatial" dimension, and not fully exploiting the spatiotemporal relations in the data and latent space as an image-to-video forecasting formulation.

The problem of image-to-video forecasting, also known as video synthesis, has been approached previously by researchers in the field of computer vision [61–65]. Iliadis et al. [66] are one of the first to develop a deep learning-based framework for video compressive sensing to reconstruct a video sequence from a single measured frame using a deep fully-connected neural network, or artificial neural network (ANN). Despite excellent accuracy in the video predictions, this method is still limited by time-distributed fully-connected layers in the encoder and decoder portions of the network, thus not exploiting the spatiotemporal relationships in the data. Xu and Ren [67] develop a three-part encoder-recurrent-decoder network for video

reconstruction from the estimated motion fields of the encoded frames. The implementation is similar to that of [17, 59, 60] in that it applies a recurrent update in the latent space but relies on time-distributed deconvolutions for the video frames reconstruction to exploit spatiotemporal relationships in the data. Dorkenwald et al. [68] develop a conditional invertible neural network (cINN) as a bijective mapping between image and video domains using a dynamic latent representation. The cINN architecture allowed for video-to-image and image-to-video predictions, proving possible the generation of video frames from a static input image. Finally, Holynski et al. [69] implemented the idea of Eulerian motion fields to define the moving portions of the image and thus were the able to accurately reconstruct a series of video frames from a static image using a spatiotemporal latent space parameterization. These advancements in the field of computer vision and video compressed sensing serve as a foundation for our image-to-video proxy model.

We propose the Stochastic pix2vid, a novel image-to-video spatiotemporal proxy model for the prediction of dynamic reservoir behavior over time from a suite of static geologic realizations representing a subsurface uncertainty model. Our model exploits the spatial and temporal structures in latent space to dynamically reconstruct the time-dependent pressure and saturation states from a static geologic realization. The encoder portion of the network receives as inputs the static geologic realization with geological depositional, high permeability channels representing the porosity, permeability, and facies spatial distributions, and the location of CO_2 injection well(s). The model then reconstructs the dynamic pressure and saturation distributions using a spatiotemporal decoder network with convolutional long short-term memory (ConvLSTM) layers, which are concatenated with the residuals of the spatial latent parameterizations from the encoder network. Thus, it is not an encoder-recurrent-decoder architecture, but instead a fully spatiotemporal convolutional-recurrent image-to-video synthesis model. Our stochastic pix2vid model shows significant advantages compared to image-to-image and encoder-recurrent-decoder models in terms of computational efficiency and prediction accuracy and can be used as a replacement for high-fidelity simulations (HFS) in GCS projects as an image-to-video mapping operator.

In the methodology section, we discuss the proposed spatiotemporal proxy model architecture as well as the geologic modeling and numerical reservoir simulation steps required to generate the training data. In the results and discussion sections, we evaluate the training and performance of the proposed proxy model and compare its efficiency and accuracy to high-fidelity numerical simulations using a 2D synthetic case for large-scale GCS operations.

2 Methodology

This section describes the governing equations, reservoir model and simulation specifications, and the architecture and training strategy of the Stochastic pix2vid model.

2.1 Governing equations For the CO_2-water multiphase flow problem, the general form of the mass accumulation for component $\kappa = CO_2$ or water is given by [70]:

$$\frac{\partial M^k}{\partial t} = -\nabla \bullet F^\kappa + q^\kappa. \tag{1}$$

For each component κ, the mass accumulation term M^κ is summed over all phases p,

$$M^k = \phi \sum_p S_p \rho_p X_p^\kappa \tag{2}$$

where ϕ is the porosity, S_p is the saturation of phase p, ρ_p is the density of phase p, and X_p^κ is the mass fraction of component κ present in phase p. For each component κ, there is also the advective mass flux $F^\kappa|_{adv}$ obtained by summing over all phases p,

$$F^\kappa|_{adv} = \sum_p X_p^\kappa F_p \tag{3}$$

where each individual phase flux F_p is given by Darcy's equation:

$$F_p = \rho_p u_p = -k \frac{k_{r,p}\rho_p}{\mu_p}(\nabla P_p - \rho_p g) \tag{4}$$

where u_p is the Darcy velocity of phase p, k is the absolute permeability, $k_{r,p}$ is the relative permeability of phase p, μ_p is the viscosity of phase p, and g is the gravitational acceleration constant. The relative permeability curves for the CO_2-water system are shown in Figure 4. The fluid pressure of phase p,

$$P_p = P + P_c \tag{5}$$

is given by the sum of the reference phase pressure P and the capillary pressure P_c. The numerical simulation does not include molecular diffusion or hydrodynamic dispersion for practical purposes.

2.2 Reservoir Model and Simulation

We use SGeMS [71] to construct an ensemble of realizations that is representative of various potential geologic scenarios for CO_2 storage in deep geological formations, e.g., fluvial, turbidite, and deepwater lobe systems. Using sequential Gaussian co-simulation [72], we generate a set of 1,000 random porosity (ϕ) and

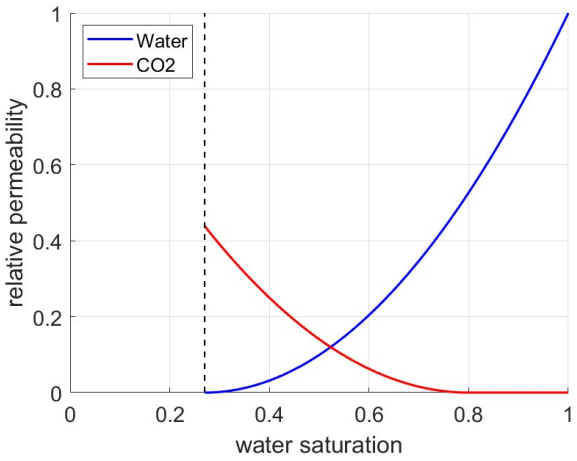

Figure 4: Relative permeability curves for the CO_2-water system. The residual saturations are 0.27 and 0.2 for water and CO_2, respectively.

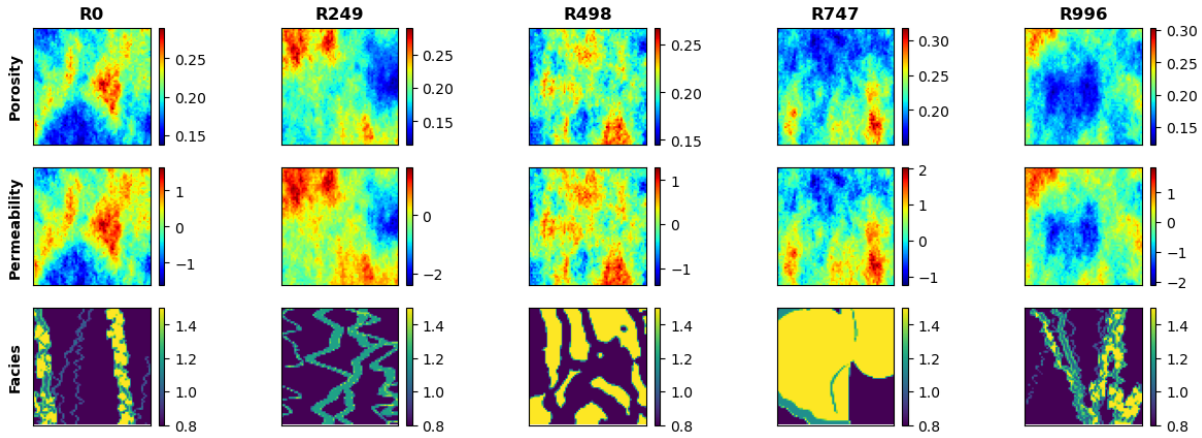

Figure 5: Spatial distribution of porosity (top), permeability (middle), and facies (bottom) for 5 random realizations.

permeability (k) distributions with a wide range of values, as shown in Figure 5. Facies distributions are obtained from a library of deepwater fluvial training images [73, 74]. These encompass a wide range of possible geologic scenarios including marked point (lobe, ellipse, and bar), FluvSim (channel, channel-levee, and channel-levee-splay), surface based (compensational cycles of lobes), and bank retreat (channel complex). To generate consistent porosity and permeability distributions with the facies-based geologic scenarios, we condition the original porosity and permeability distributions to the facies distributions. The resulting fluvial distributions are shown in Figure 6.

The conditioned fluvial porosity and permeability distributions are used as inputs for the numerical simulation of geologic CO_2 storage using MRST [75]. Specifically, the MRST-co2lab module is used as an automatic-differentiation framework for the compositional simulation of the two-phase CO_2-water problem. The reservoir is initialized as a fully water saturated zone (i.e., aquifer) with an initial pressure of 4,000 psi.

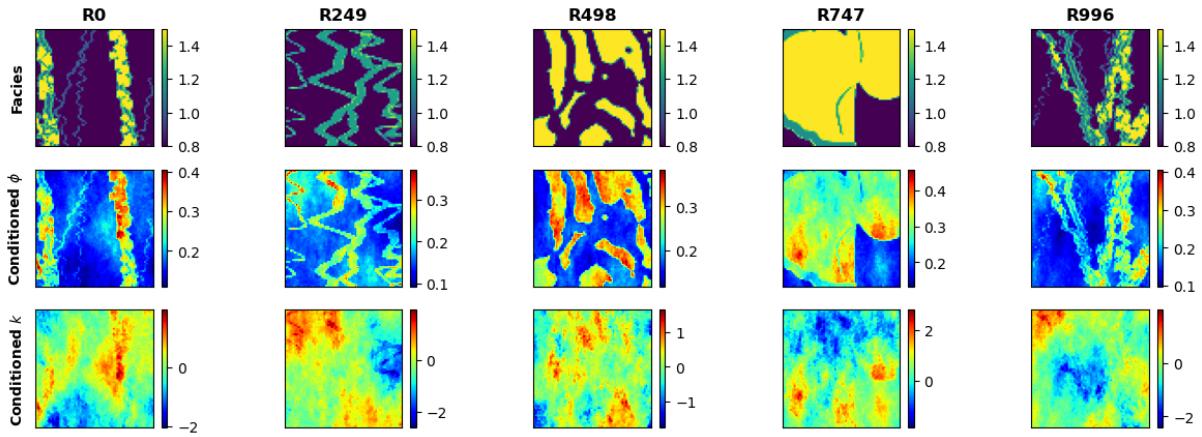

Figure 6: Spatial distribution conditioned to facies (top) for porosity (middle) and permeability (bottom) for 5 random realizations.

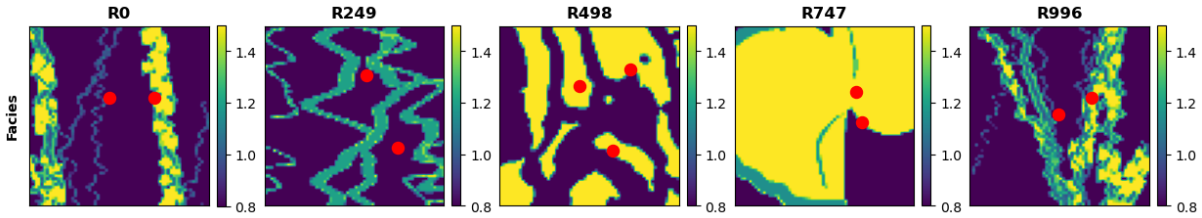

Figure 7: CO_2 injection well(s) location (red) overlaid over facies distributions for 5 random realizations.

The reservoir has constant isothermal conditions and constant pressure boundary conditions to represents a large-scale geologic CO_2 storage project with negligible dip, such as found in the Illinois Basin and parts of the North Sea and Gulf of Mexico.

The model has dimensions of 1km-1km-100m in the x-, y-, and z-directions, respectively. We use 64 uniform grid cells in the x- and y-directions. The grid design is sufficiently refined to resolve the pressure and saturation plumes in highly heterogeneous reservoirs while remaining computationally tractable for the purpose of training deep learning models. A random number of injection wells, $w \in [1, 3]$, are placed randomly along the reservoir for each of the 1,000 realizations, no closer than 250m from the boundaries, as shown in Figure 7. The injection well(s) are randomly placed and not conditioned to zones of preferential porosity, permeability, nor facies. Each injection well has a constant radius of 0.1m and a single and continuous perforation that injects pure supercritical CO_2 at a constant rate such that the total injection rate of the w well(s) is 0.5 megatons per year.

The numerical simulation is run for 5 years, monitored monthly, for a total of 60 timesteps. At each grid cell and for each time step, we resolve the implicit pressure, explicit saturation (IMPES) formulation of Eq. (1) to obtain the corresponding dynamic pressure and saturation distributions over time (videos) from

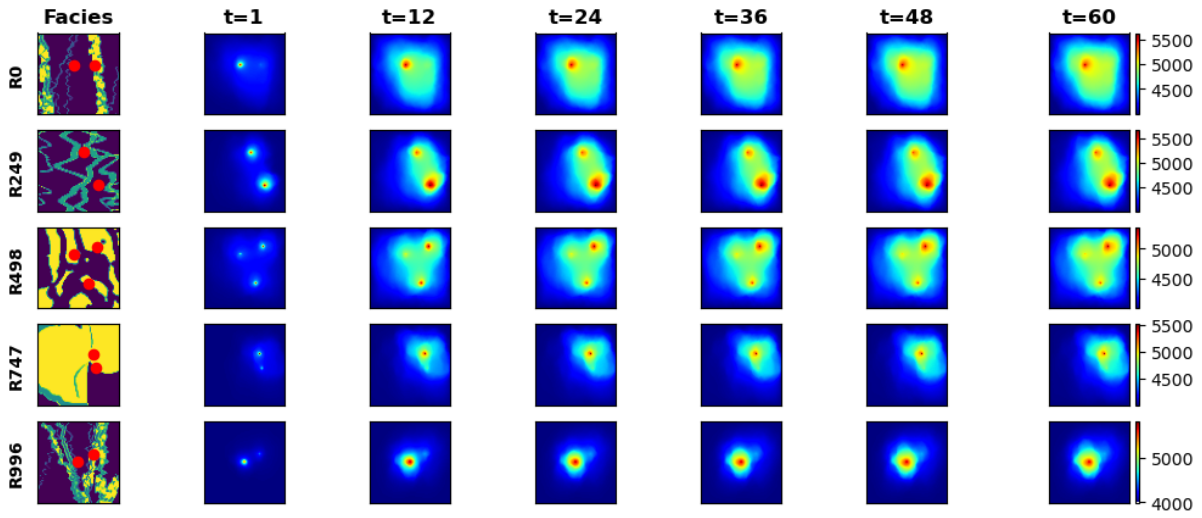

Figure 8: Pressure response distributions over time for 5 random realizations obtained from HFS (in psia).

the static geologic realizations of porosity and permeability conditioned to the fluvial facies (images) with random well(s) configuration. The pressure and saturation responses corresponding to the previously-shown geologic model realizations are shown in Figures 8 and 9, respectively.

2.3 Proxy Model Architecture

The Stochastic pix2vid model is designed as an image-to-video data-driven mapping operator from the static realizations of geologic distributions of porosity, permeability and facies as well as the injector well(s) distribution, to the dynamic responses of pressure and saturation distributions over time. A single model is trained to predict both pressure and saturation distributions over time as a multi-channel output from the multi-channel input features.

Let m represent a geologic model realization of porosity, permeability, facies, and injector well(s) distributions, such that $m = \{\phi, k, facies, w\}$. The dynamic responses of pressure and saturation over time are given by $d = f(m)$, such that $d = \{P(t), S(t)\}$ and f is the physics-based numerical reservoir simulation. Our aim is to replace f with a more efficient data-driven proxy by training the Stochastic pix2vid model. For this purpose, we exploit the latent structures in space and time of the static inputs and dynamic outputs through a spatiotemporal encoder-decoder architecture.

The encoder portion of the network is comprised of sequential convolutional layers to compress the spatial features of the model realizations into a latent parameterization z_m, given by $z_m = Enc(m)$. In their compressed representation, these features represent the salient characteristics of the geologic distributions. The decoder portion of the network is designed as a series of recursive residual convolutional-recurrent layers, such that the latent space z_m is recursively decoded into the dynamic distributions of pressure and saturation over time. The previous timestep latent representations, z_d^t, are used in the subsequent timestep to refine

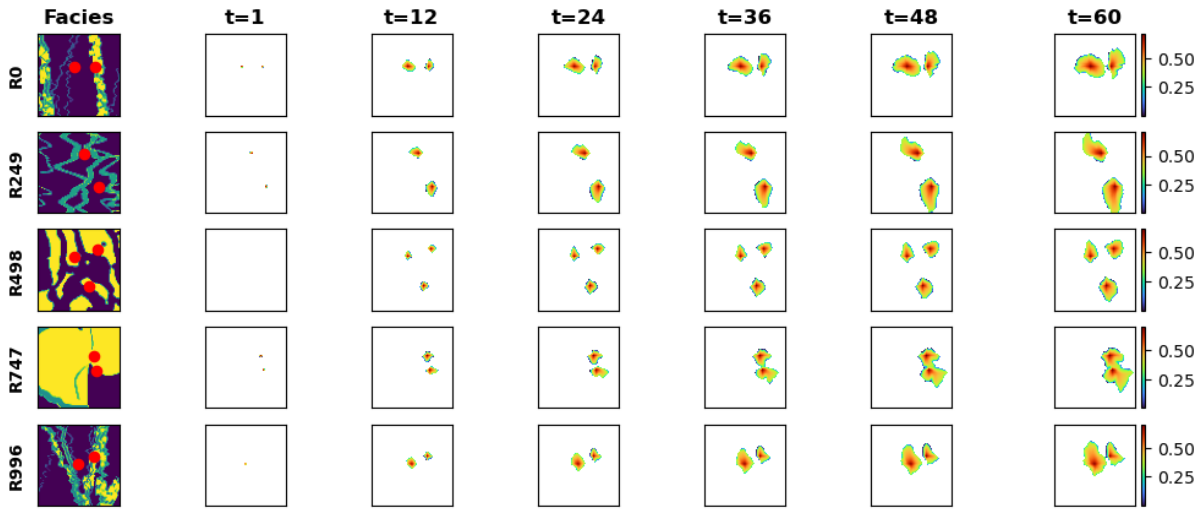

Figure 9: Saturation response distributions over time for 5 random realizations obtained from HFS.

the outputs and reduce systematic error propagation in time. Thus, the full architecture is represented as

$$\hat{d} = Dec^t([Enc(m); z_d^t]) \tag{6}$$

The encoder portion compresses the geologic realizations, m, into a latent representation z_m through the use of depthwise separable convolutions [76]. This type of convolution learns the parameters for each channel in the image separately, avoiding mixing of variables or loss of resolution, as shown in Figure 10. This is especially important when dealing with Gaussian-distributed permeability and porosity in combination with binomial-distributed facies and binary well(s) location distributions. Each separable convolution layer is regularized with an l_1-norm weight of 1×10^{-6} to control the null space in latent feature space. Moreover, we use a Squeeze-and-Excite layer to improve channel interdependence, and to avoid mixing and loss of resolution [77]. Each Squeeze-and-Excite layer will provide the optimal network weights for each channel independent of the other channels by passing the feature maps through a global pooling layer (squeeze) and a dense layer with nonlinear activation (excite), to add content aware mechanism for re-weighting each channel adaptively, as shown in Figure 11. Furthermore, by applying instance normalization, as opposed to the more common batch normalization, we achieve channel-independent normalization of the convolved features [78]. Instance normalization is a special case of group normalization, where the numbers of channels per group is exactly 1, such that each channels gets its own normalization scheme, as shown in Figure 12. Parametric rectified linear units (PReLU) is used as the activation function, where at each minibatch iteration, the network learns the optimal leaky slope for activation in each layer, as shown in Figure 13. Finally, pooling and spatial dropout are applied, as the resulting feature map is reduced to half the input dimension. Through

3 convolutional encoding layers with filter size 3×3, we obtain the latent parameterizations z_m^1, z_m^2, and z_m^3. Table 1 summarizes the architecture and dimensions of each layer.

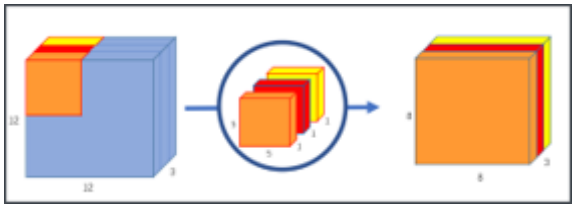

Figure 10: Schematic for a separable convolutional layer. Each channel is convolved with its own set of convolutional filters to obtain the best representation, as opposed to traditional convolutions where the same filter is applied to all channels in the data.

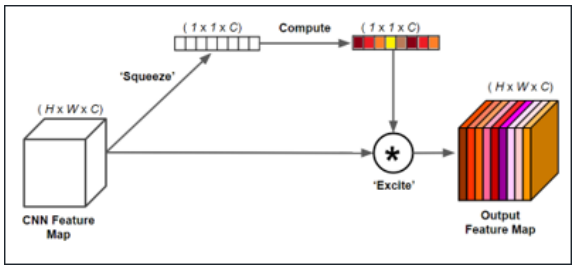

Figure 11: Schematic for a squeeze-and-excite layer. The "squeeze" layer takes the global average of the data for each channel, and the "excite" layer is a fully-connected layer with nonlinear activation to estimate the optimal weights for each channel in the data. The result is a weighted representation of the data based on their intrinsic global characteristics.

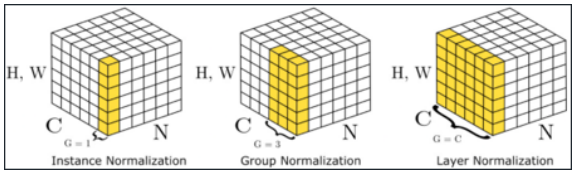

Figure 12: Schematic for instance normalization (left) compared to group normalization (center) and batch normalization (right). In an instance normalization layer, each channel will be normalized by themselves rather than normalizing the entire batch or a subset of channels (groups).

The decoder portion of the Stochastic pix2vid model extracts the spatiotemporal relationships from the latent representations of m to reconstruct the dynamic pressure and saturation distributions over time, d. To accurately reconstruct the spatiotemporal structure from the static latent space, z_m, we employ a series of convolutional-recurrent layers, namely a convolutional long-short term memory layer (ConvLSTM). The general form of a 2D ConvLSTM layer is shown in Figure 14. Through 3 convolutional-recurrent layers, we obtain the dynamic prediction of d as follows:

Step 1: **Spatiotemporal decoding of** z_m^3: The first ConvLSTM layer takes the smallest latent representation, z_m^3, and reconstructs the first decoded timestep z_d^3.

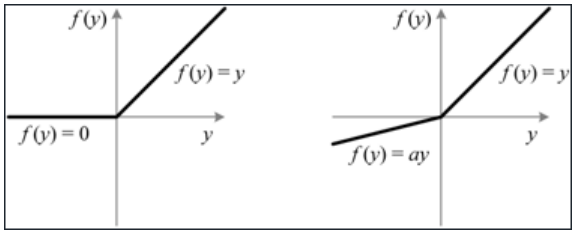

Figure 13: Schematic for the Parametric Rectified Linear Unit (PReLU) activation function (right) compared to the traditional ReLU activation function (left). The slope of the negative portion of the data, α, is learned for each batch.

Table 1: Encoder network architecture

Layer Number	**Architecture**	**Shape in** (h,w,c)	**Shape out** (h,w,c)
1	SeparableConv2D Squeeze-and-Excite Instance Norm PReLU + Pooling Spatial Dropout	$64 \times 64 \times 4$ (m)	$32 \times 32 \times 64$ (z_m^1)
2	SeparableConv2D Squeeze-and-Excite Instance Norm PReLU + Pooling Spatial Dropout	$32 \times 32 \times 64$	$16 \times 16 \times 128$ (z_m^2)
3	SeparableConv2D Squeeze-and-Excite Instance Norm PReLU + Pooling Spatial Dropout	$16 \times 16 \times 128$	$8 \times 8 \times 256$ (z_m^3)

Step 2: **Residual concatenation of** z_m^2: The first decoded timestep, z_d^3, is concatenated with the intermediate static encoding z_m^2 to retain multi-scale features and improve prediction performance and resolution.

Step 3: **Intermediate spatiotemporal decoding**: The second ConvLSTM layer takes the residual concatenation of the intermediate latent representations, $[z_m^2, z_d^3]$, to predict the next spatiotemporal representation z_d^2.

Step 4: **Residual concatenation of** z_m^1: The intermediate decoded timestep, z_d^2, is concatenated with the largest static encoding z_m^1.

Step 5: **Final spatiotemporal decoding**: The third ConvLSTM layer takes the residual concatenation of the larger latent representations, $[z_m^1, z_d^2]$, to predict the full-scale dynamic output, d.

To enhance the performance of the spatiotemporal decoding, each ConvLSTM layer is followed by a batch

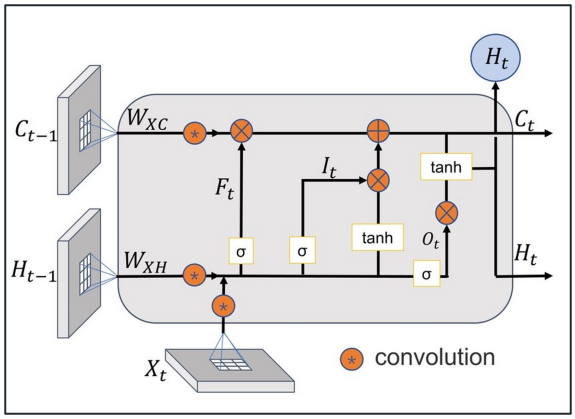

Figure 14: Schematic of a convolutional-LSTM (ConvLSTM) layer. The layer applies convolutional operations to the input data using a set of learnable filters to capture the spatial patterns. The recurrent part is a long short-term memory layer with memory and forget gates to capture the temporal patterns. LSTM units are applied to each spatial location separately allowing to capture both spatial and temporal dependencies in the data.

normalization, activation, and a transpose convolutional layer, the latter for downscaling the latent features to twice their dimension. Spatial dropout is applied, and the concatenated features are once more convolved and activated to obtain the layer prediction. Table 2 shows the architecture of the decoder network.

This process yields the first video frame prediction, d_1, from the latent representation of the geologic realizations z_m. Each subsequent video frame prediction is obtained by another set of residual concatenation of the previous timestep dynamic decoded representation. The static latent representation z_m is concatenated at each timestep with the previous dynamic decoded representation for each layer such that we have $[z_m, z^i_{d_t}]$, where i is the decoding layer number and t is the timestep. By recursively implementing spatiotemporal decoding to the latent representation z_m, we obtain the prediction of the dynamic response d_t at times for each timestep $t = 1, \ldots, n$.

The complete Stochastic pix2vid architecture is shown in Figure 15. Here we observe the spatial compression of the geologic models, m, through the encoding portion of the network, and the spatiotemporal decoding and residual multi-scale concatenations through the decoder portion of the network. The resulting architecture provides proxy model from static geologic models (images) to dynamic reservoir response (videos).

2.4 Training Strategy

The inputs to the Stochastic pix2vid are the geologic realizations, comprised of the distributions of porosity, permeability, facies, and injection well(s) location, represented as a matrix m of dimensions $64 \times 64 \times 4$. The outputs are the results from the numerical reservoir simulation, namely pressure and saturation distributions over time, represented as a matrix d of dimensions $64 \times 64 \times 60 \times 2$. This yields an ill-posed

Table 2: Decoder network architecture

Layer Number	**Architecture**	**Shape in** (t,h,w,c)	**Shape out** (t,h,w,c)
1	ConvLSTM2D BatchNorm + LeakyReLU Conv2DTranspose Spatial Dropout Concatenate (z_m^3) Conv2D + Sigmoid	$1 \times 8 \times 8 \times 256$	$t \times 16 \times 16 \times 128$ ($z_{d_t}^3$)
2	ConvLSTM2D BatchNorm + LeakyReLU Conv2DTranspose Spatial Dropout Concatenate (z_m^2) Conv2D + Sigmoid	$t \times 16 \times 16 \times 128$	$t \times 32 \times 32 \times 64$ ($z_{d_t}^2$)
3	ConvLSTM2D BatchNorm + LeakyReLU Conv2DTranspose Spatial Dropout Concatenate (z_m^1) Conv2D + Sigmoid	$t \times 32 \times 32 \times 64$	$t \times 64 \times 64 \times 2$ ($z_{d_t}^1$)

and under-determined estimation problem, which are known to be difficult to resolve [79, 80]. To improve the training efficiency and performance, we subsample in time from 60 timesteps to 11. In other words, instead of monthly monitoring, we predict the dynamic outputs at the initial step and every 6 months afterward; therefore the output matrix d a final dimension of $64 \times 64 \times 11 \times 2$. We also perform min-max normalization so that the input and output features are in the range of $[0, 1]$, which greatly improves the performance of the nonlinear activation functions. Furthermore, we perform data augmentation by 90° rotation, making the network agnostic to orientation and effectively learning the flow physics in the system rather than memorizing spatial distribution patterns. The total amount of training data is therefore 2,000 realizations (after augmentation), which is split into 1,500 realizations for training and 500 realizations for testing. To improve model generalizability, at each epoch, each minibatch is split into 80/20 for training and validation sets, respectively.

A custom three-part loss function is used to accurately predict pixel-wise and perceptual information in the predictions. The mean squared error (MSE) is used to reconstruct the pixel-wise intensity values, while the mean absolute error (MAE) is used to optimize for the pressure and saturation plume edges. The third part is the structural similarity index metric (SSIM), which provides a perceptual image-to-image comparison of luminance, contrast, and structure [81]. For optimal training, the aim is to minimize the MSE and MAE while maximizing the SSIM for the true versus predicted outputs, d and $\hat{d}$, such that the total loss is given by:

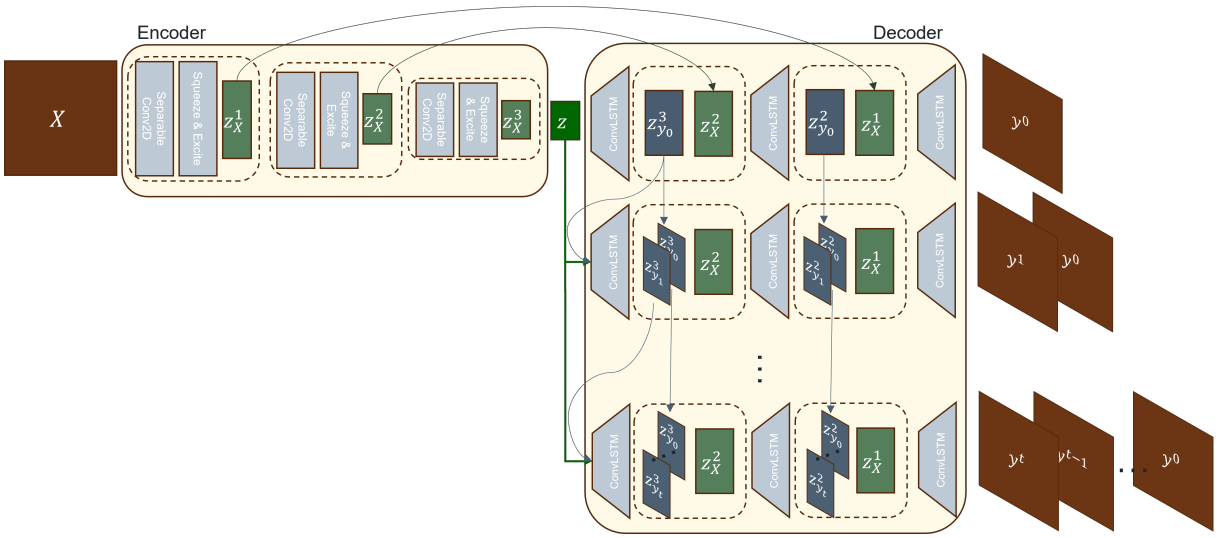

Figure 15: Architecture of the Stochastic pix2vid model. The input data, $X \equiv m$, is encoded through a series of convolutional layers to capture the spatial dependencies in the geologic models. The latent representation, z_m, is recursively passed through a spatiotemporal decoder with convolutional-recurrent layers, and concatenated with the residuals of the encoder to reconstruct iteratively the frames of the output (video) data, $y \equiv d$.

$$\mathcal{L} = \alpha(1 - SSIM) + (1 - \alpha)[\beta MSE + (1 - \beta)MAE] \tag{7}$$

where α and β are weighting coefficients obtained empirically as 0.33 and 0.66, respectively.

The model is trained using the AdamW optimizer [82]. This variant of the well-known adaptive momentum (Adam) optimizer [83] includes an added method to decay weights for the adaptive estimation of first-order and second-order moments. We implement a learning rate of 1×10^{-3} with a weight decay term of 1×10^{-5}.

3 Results

This section describes the Stochastic pix2vid model training performance and discusses the application of the proxy to rapidly forecast CO_2 plume migration for a large-scale GCS operation.

3.1 Training Performance

Using an NVIDIA Quadro M6000 GPU, we train for 100 epochs with a batch size of 50. The model has a total of 97,523,370 parameters, and the training time required is approximately 88 minutes for all 1,500 training realizations. The training and validation performance per epoch is shown in Figure 16. We observe minimal overfit in the validation set, corresponding to good model generalizability and prediction accuracy within the training data. Using physics-based numerical simulation, each realization requires approximately

30 seconds to obtain the dynamic pressure and saturation predictions from the static geologic models. Our Stochastic pix2vid model obtains the same results in approximately 4.59 milliseconds, corresponding to a 6,500× speedup. The average MSE for the ensemble is 9.21×10^{-4} and 9.70×10^{-4} for training and testing, respectively. Similarly, the average SSIM for the ensemble is 98.97% and 97.91% for training and testing, respectively.

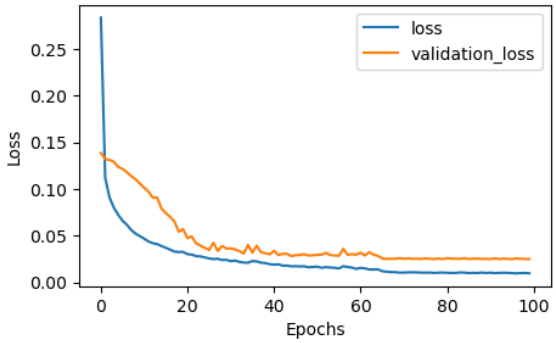

Figure 16: The total training and validation losses, $\mathcal{L}$, as a function of epoch number.

3.2 Prediction Results

After training the Stochastic pix2vid model with 1,500 realizations of static geologic models, $m = \{\phi, k, facies, w\}$, to predict the dynamic reservoir response, $d = \{P(t), S(t)\}$, we can compare the performance of the predictions for the training and unseen testing data.

Figures 17 and 18 show the predicted dynamic pressure and saturation distributions, respectively, along with the absolute difference to HFS for 3 training realizations. We observe reasonable agreement between the true and predicted CO_2 pressure and saturation plumes over time, with an average MSE of 3.25×10^{-4} and SSIM of 98.59% for pressure predictions and MSE of 1.50×10^{-4} and SSIM of 97.31% for saturation predictions.

Similarly, Figures 19 and 20 show the pressure and saturation distributions predictions along with the absolute difference to HFS for 3 testing realizations. We observe a similar performance, with an average MSE of 3.71×10^{-4} and SSIM of 97.55% for pressure predictions and MSE of 1.61×10^{-3} and SSIM of 96.19% for saturation predictions. This indicates that the Stochastic pix2vid model has excellent generalization ability and achieves on par performance with HFS at a fraction of the computational cost.

It is interesting to note that the Stochastic pix2vid model is trained on a triple-loss function with MSE, MAE and SSIM. For both training and testing cases, we see that the average MSE for pressure is higher than that of saturation, while the opposite is true for the average SSIM. This can be attributed to the fact that there are more pixel-wise variations in pressure predictions, thus the loss focuses on matching those individual pixel-wise values. On the other hand, for saturation predictions, the contrast, luminance, and

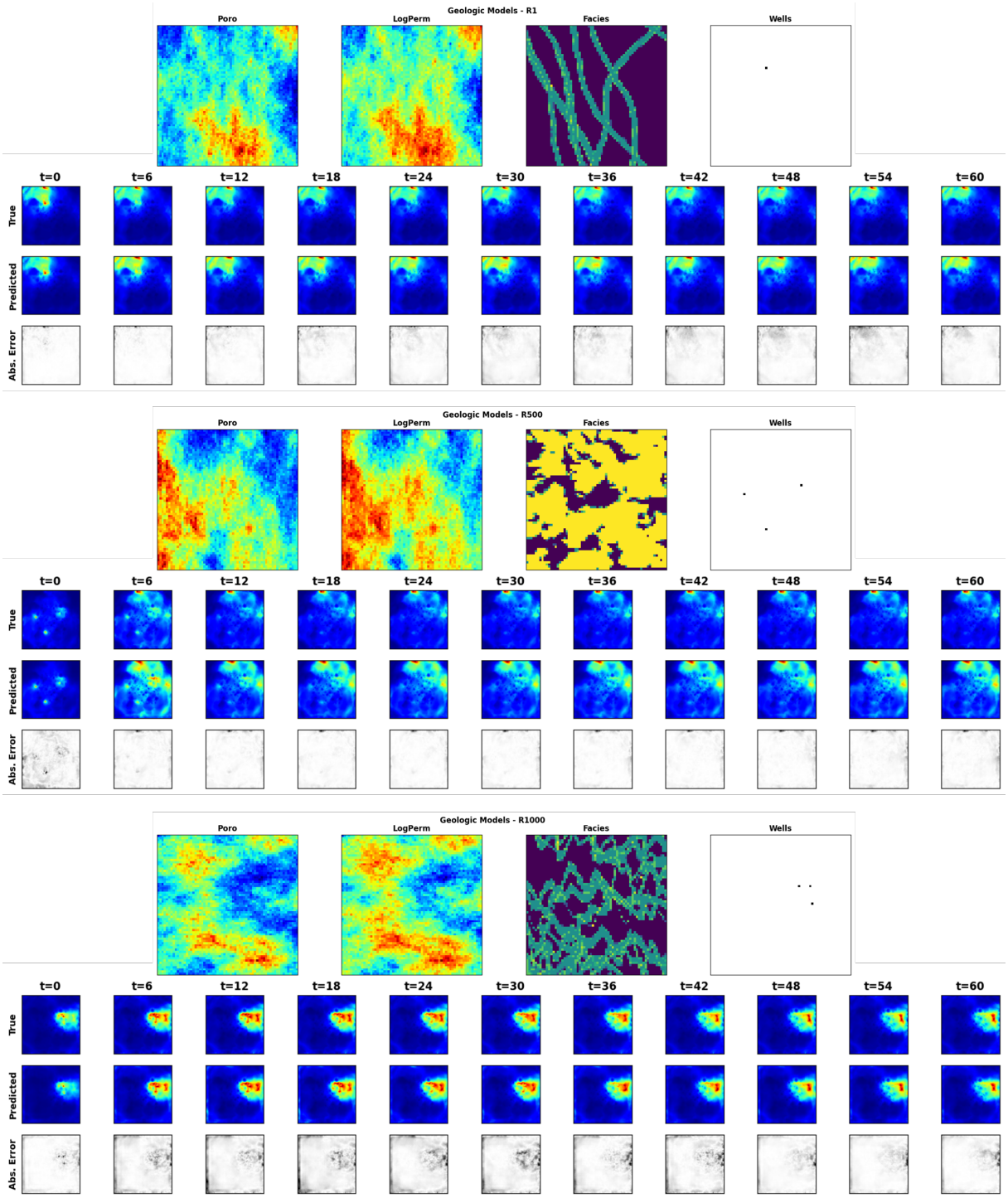

Figure 17: (Normalized) pressure distribution over time for 3 random training realization. For each panel, the top row is the ground truth from the HFS, the middle row is the Stochastic pix2vid prediction, and the bottom row is the absolute difference to HFS.

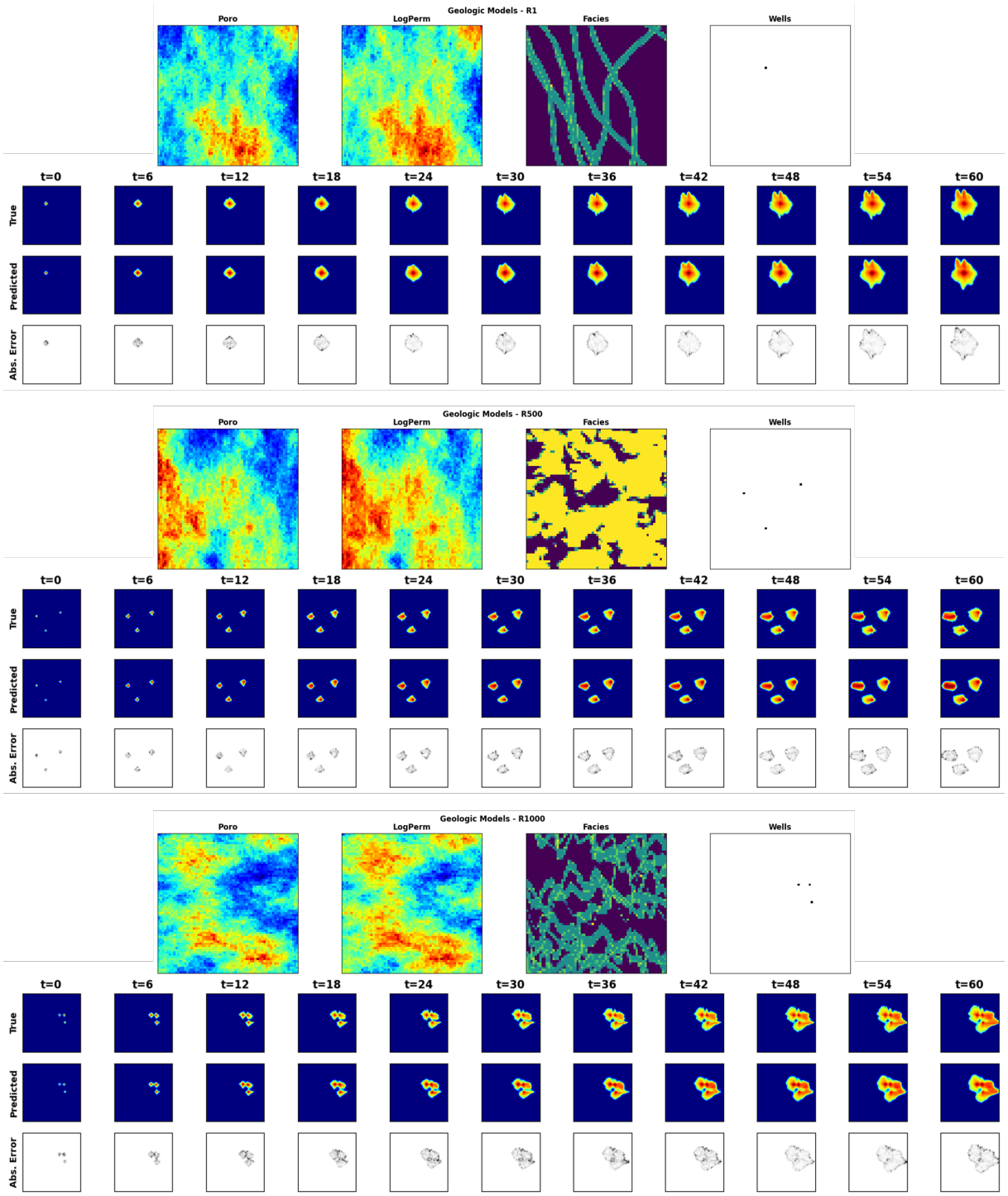

Figure 18: Saturation distribution over time for 3 random training realization. For each panel, the top row is the ground truth from the HFS, the middle row is the Stochastic pix2vid prediction, and the bottom row is the absolute difference to HFS.

structure play a bigger role in the prediction that the pixel-wise intensity values. Therefore, it is important to take into account both metrics for training and validating spatiotemporal subsurface prediction models.

From **Section 2.3**, the first step of the Stochastic pix2vid model is to take the static geologic realizations, m, and compresses them into a latent space representation, z_m, using the spatial encoder structure. Figure 21 show a random selection of latent feature maps, along with their superposition on the porosity and facies distribution. This can be interpreted as an analog to the attention head mechanisms recently developed in transformer-based architectures [84]. We observe that the latent feature maps are essentially learning the injection location(s) and direction of flow based on the geologic distributions. Thus, proving that the Stochastic pix2vid model is learning multiphase flow physics and dynamic reservoir behavior appropriately.

These results imply that our Stochastic pix2vid is capable of learning the spatiotemporal relationship between the static geologic models and the dynamic reservoir response. Thus, our image-to-video architecture can outperform current image-to-image and encoder-recurrent-decoder architectures to provide improved reservoir behavior prediction closer to that of conventional numerical simulation. To quantify the uncertainty in predictions, a comparison of true (d) versus predicted ($\hat{d}$) response for pressure and saturation distributions for the testing data is shown in Figure 22. The average R^2 over time is approximately 99% with narrow 95% prediction bands that recursively narrow over time. From Figure 22 we observe the advantage in implementing recursive refining of predictions over time with recurrent residual connections in the spatiotemporal decoder network, thus reducing the spatiotemporal uncertainty in the predictions.

CO_2 saturation and pressure buildup fronts are important quantities for geologic CO_2 storage projects and are often used for regulatory oversight [85, 86], monitoring metrics or history matching purposes [87, 88]. The distance between the injection well(s) and the saturation fronts represents the maximum extent of the CO_2 plume; however, these are often very difficult to capture accurately with data-driven proxy models. Our Stochastic pix2vid model shows greater absolute error on and around the plume fronts compared to within the plumes. However, the overall shape and intensity of the pressure and saturation distributions over time is very well captured for all realizations despite being highly heterogeneous. Therefore, the Stochastic pix2vid model can be used as a reliable replacement for expensive numerical reservoir simulations, especially in cases where large number of runs are required to obtain dynamic estimates (e.g., well placement and control optimization, history matching, uncertainty quantification).

3.3 Discussion

In our Stochastic pix2vid model, the encoder block is composed of separable convolutions, squeeze and excite layers, and instance normalization. These three particular implementations allow for precise parameterization of the geologic realization into a latent representation, without mixing the effects of Gaussian-distributed properties against binary of binomial-distributed properties. Using recursive residual ConvLSTM

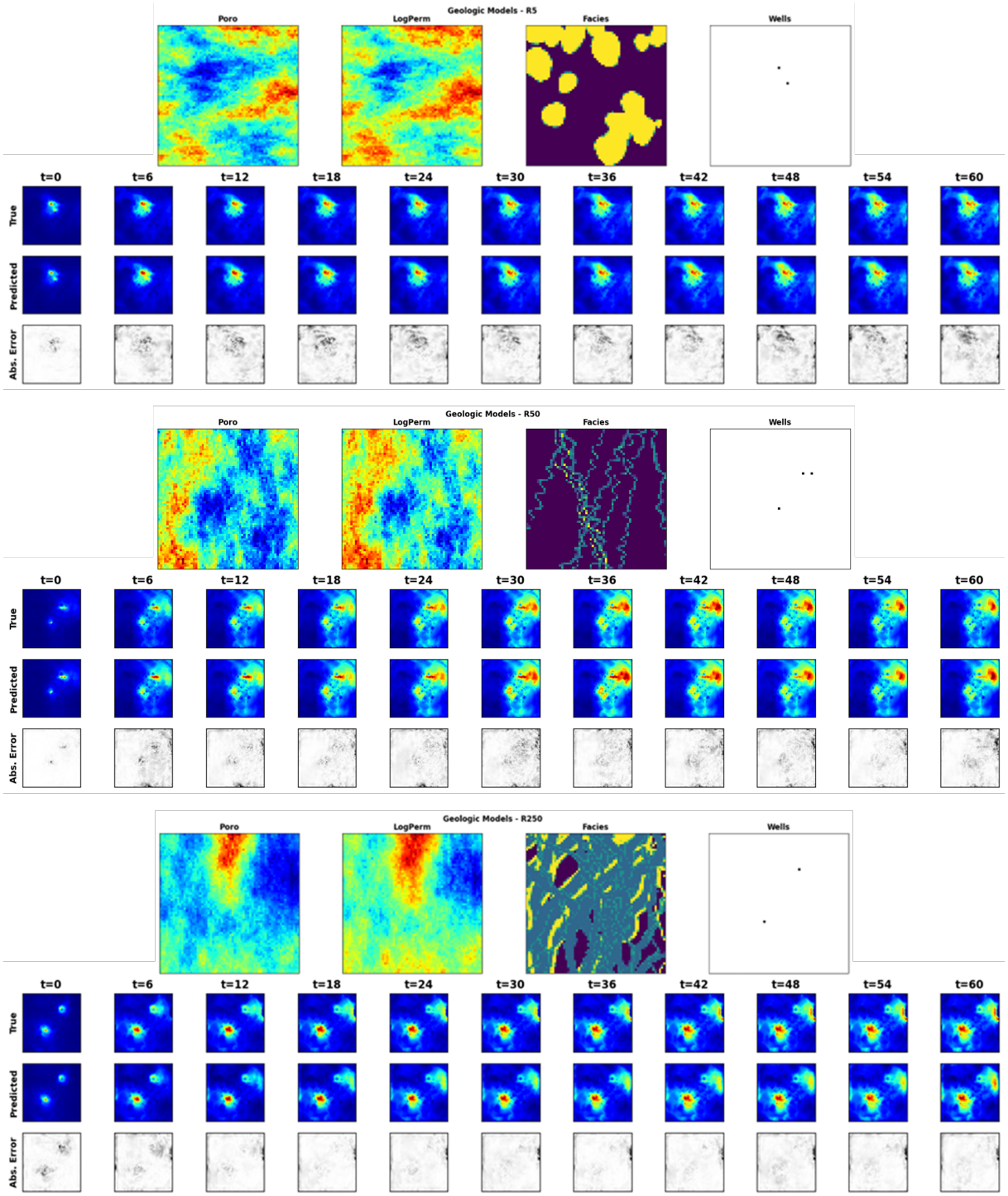

Figure 19: (Normalized) pressure distribution over time for 3 random testing realization. For each panel, the top row is the ground truth from the HFS, the middle row is the Stochastic pix2vid prediction, and the bottom row is the absolute difference to HFS.

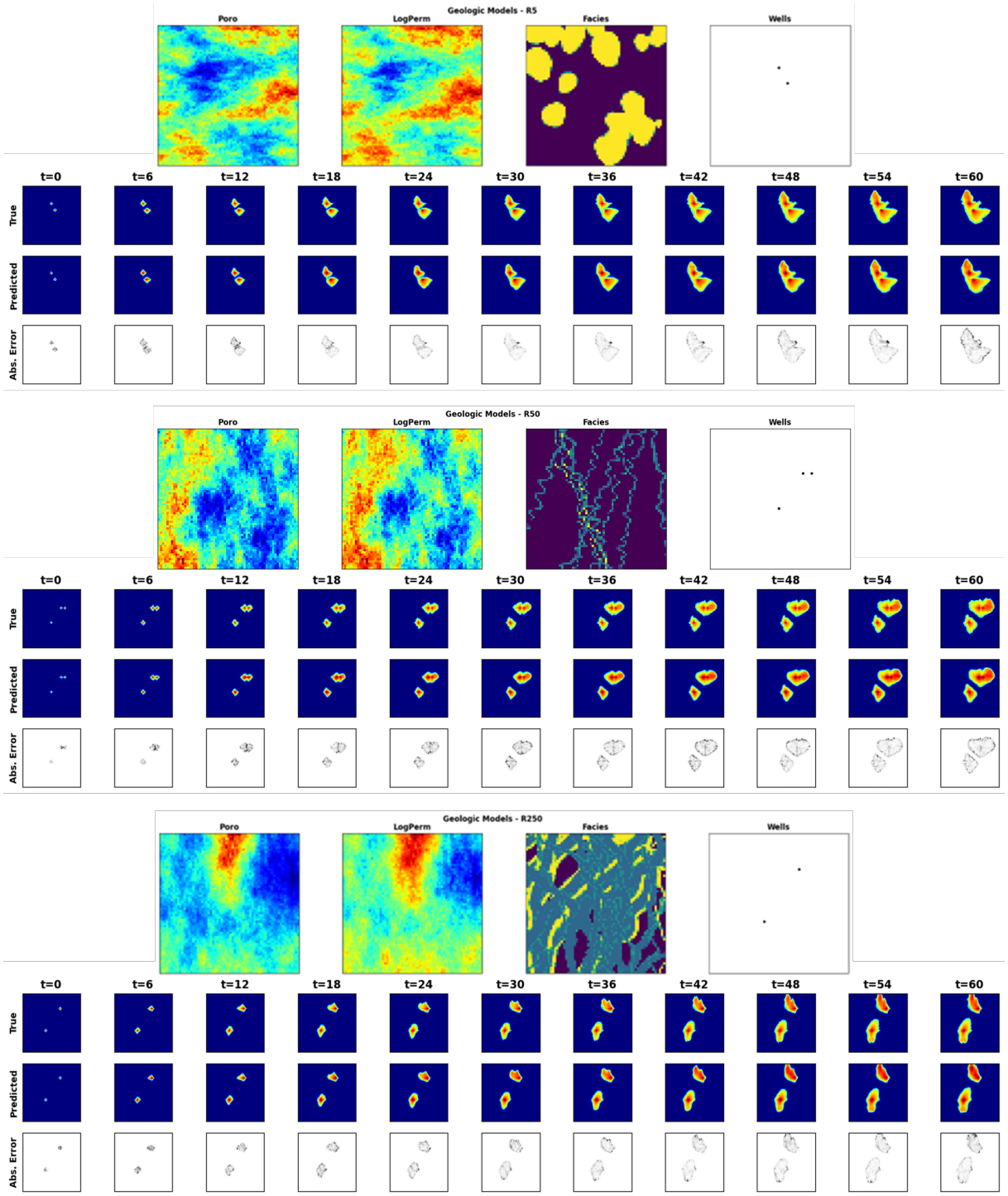

Figure 20: Saturation distribution over time for 3 random testing realization. For each panel, the top row is the ground truth from the HFS, the middle row is the Stochastic pix2vid prediction, and the bottom row is the absolute difference to HFS.

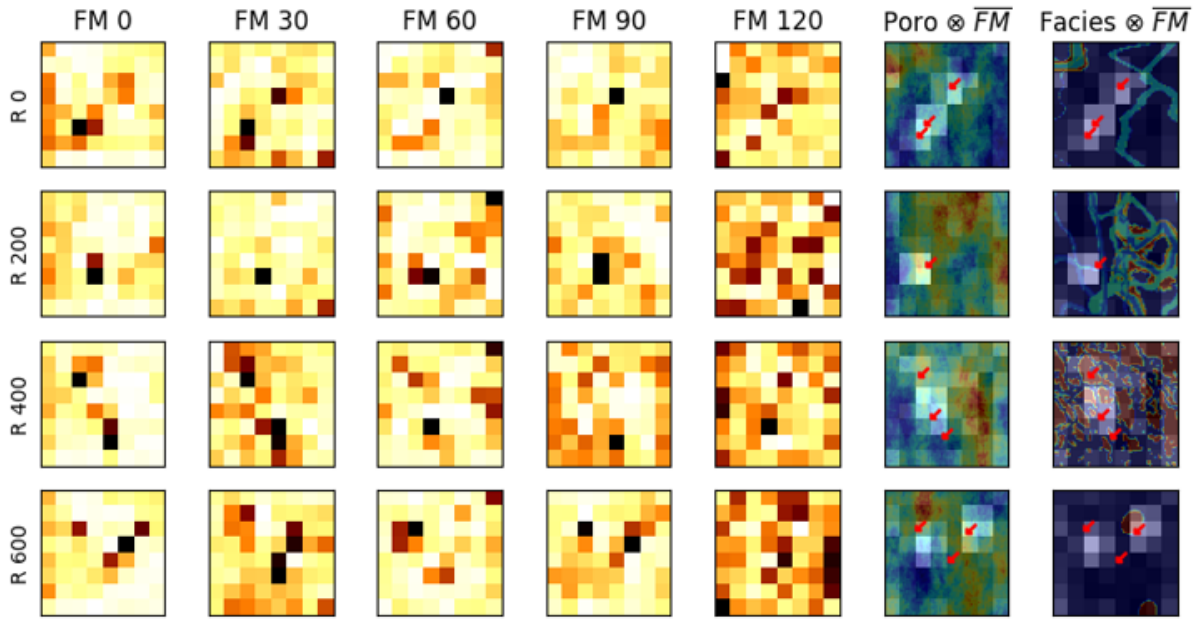

Figure 21: Five random feature maps (FM) of z_m^3 for 4 random realizations. Their average is overlaid on top of the porosity and facies distributions to show the attention mechanism of the encoder. Bright colors represent higher attention and dark colors represent lower attention.

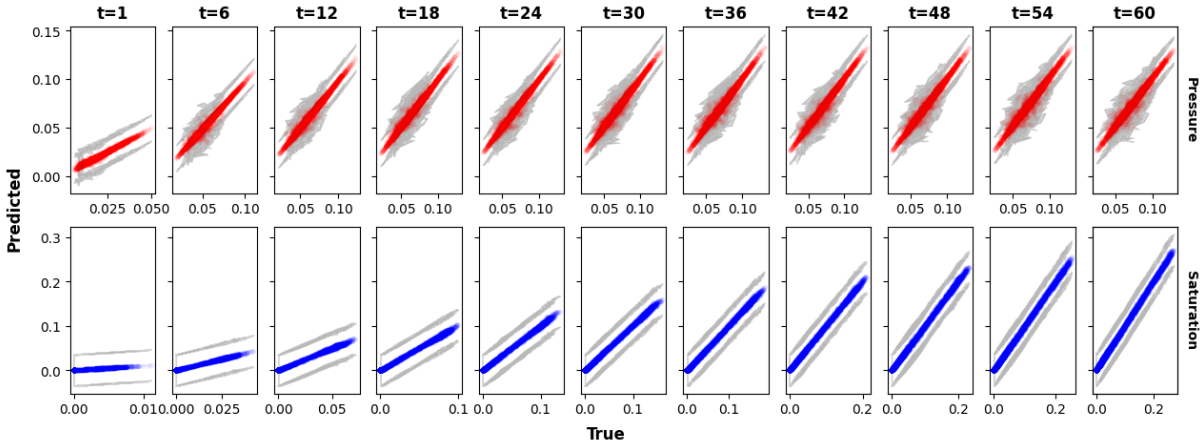

Figure 22: True versus predicted average (normalized) pressure (top) and saturation (bottom) over time for the testing data. The gray portion represents the 95% confidence bands, which become narrower over time.

layers, the decoder block iteratively predicts each dynamic state, or video frame, from the concatenation of the previous dynamic latent representation and the intermediate encoding parameterizations. Thus, our architecture makes the proxy model an image-to-video prediction formulation for dynamic reservoir states from a static geologic realization.

By using GPU-enabled computations, we significantly accelerate the training and prediction time of the Stochastic pix2vid model. Each HFS run was performed on an Intel ®i9-10900KF processor with 10 cores. The 1,000 realizations are parallelized equally among all cores and the total simulation time accounting for parallelization for all realizations is about 8.33 hours. Dynamic prediction of the 1,000 realizations using the Stochastic pix2vid model on an NVIDIA Quadro M6000 GPU require a total of 4.6 seconds, or 0.001275 hours, with an accuracy of 99% and 98% for training and testing, respectively. This provides a sustainable argument for the usage of our Stochastic pix2vid model as a replacement for HFS when computational time is a constraint.

To further demonstrate the effectiveness of our Stochastic pix2vid model for geologic CO_2 storage operations, we plot the cumulative pixel-wise CO_2 saturation as a surrogate for the cumulative CO_2 volume injected. For all training and testing realizations, Figure 23 shows the sum of pixel-wise CO_2 saturation and the probability density function (PDF) of the true versus predicted saturations. We observe an R^2 of 98% for training and 96% for testing in the cumulative CO_2 saturation of true versus predicted results, and a conformable PDFs for both training and testing.

4 Conclusions

We develop a deep learning-based spatiotemporal proxy model to provide flow predictions for a large-scale GCS operation. The key extension introduced is the use of a spatiotemporal convolutional-recurrent architecture for dynamic predictions of CO_2 pressure and saturation distributions over time from a static geologic realization representing the subsurface uncertainty model. The framework is developed as an image-to-video prediction, which is an under-determined estimation problem. Specifically, the implementation expands upon the architectures of current encoder-recurrent-decoder models and provides a fast and accurate proxy as a replacement for physics-based numerical reservoir simulation.

The spatiotemporal proxy is applied to a synthetic 2D GCS project with multiple uncertain geologic scenarios and random number and location of injection well(s). A total of 1,000 geologic models are obtained from a variety of possible geologic scenarios including fluvial, turbidite, and deepwater lobe systems. The spatial distribution of porosity, permeability and facies, and the spatial location of the injector well(s) are used as the input data. The proxy model is used to predict the dynamic reservoir response over time, namely the

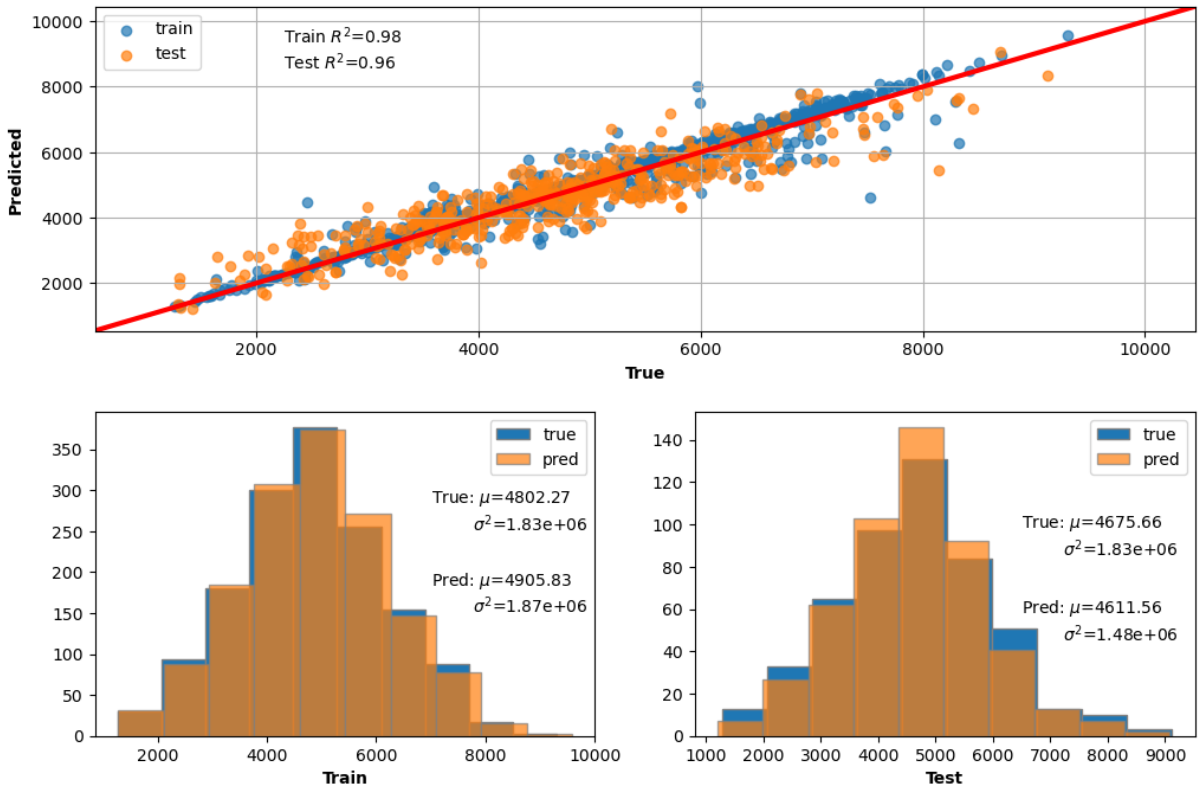

Figure 23: (Top) True vs. predicted cumulative CO_2 volume injected via pixel-wise saturation. (Bottom) True vs. predicted distributions of cumulative CO_2 saturation for training (left) and testing (right).

video frames, corresponding to the dynamic CO_2 pressure and saturation distributions, which are obtained offline for training using HFS. The total training time is 88 minutes on a single NVIDIA Quadro M6000 GPU, and predictions are obtained with 98-99% accuracy within approximately 4.6 milliseconds, compared to the approximate 30 seconds required for HFS – a $6,500\times$ speedup.

There are several possible directions that could be considered for future work. First, an extension to 3D geologic models and their corresponding dynamic predictions is key to scaling up this method for real-world applications. Similarly, although the Stochastic pix2vid proxy model was only trained for GCS prediction, it is applicable for a range of processes such as compositional, geothermal, or conventional oil and gas systems. Moreover, it is possible to extend the Stochastic pix2vid model from a data-driven mapping operator to a PINN by including the discretized form of the governing PDE in the loss function and minimizing the residuals. Another future direction would be to test the performance of the Stochastic pix2vid model on unseen timesteps, either interpolating the training timesteps or extrapolating beyond the training timesteps. Furthermore, the Stochastic pix2vid model can be used as a proxy in workflows for history matching and closed-loop reservoir management.

Reproducibility

The code will be made publicly available on the author's repository (github.com/misaelmmorales and github.com/GeostatsGuy).

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Declarations

The authors declare no conflict of interests.

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